Original bias Slides

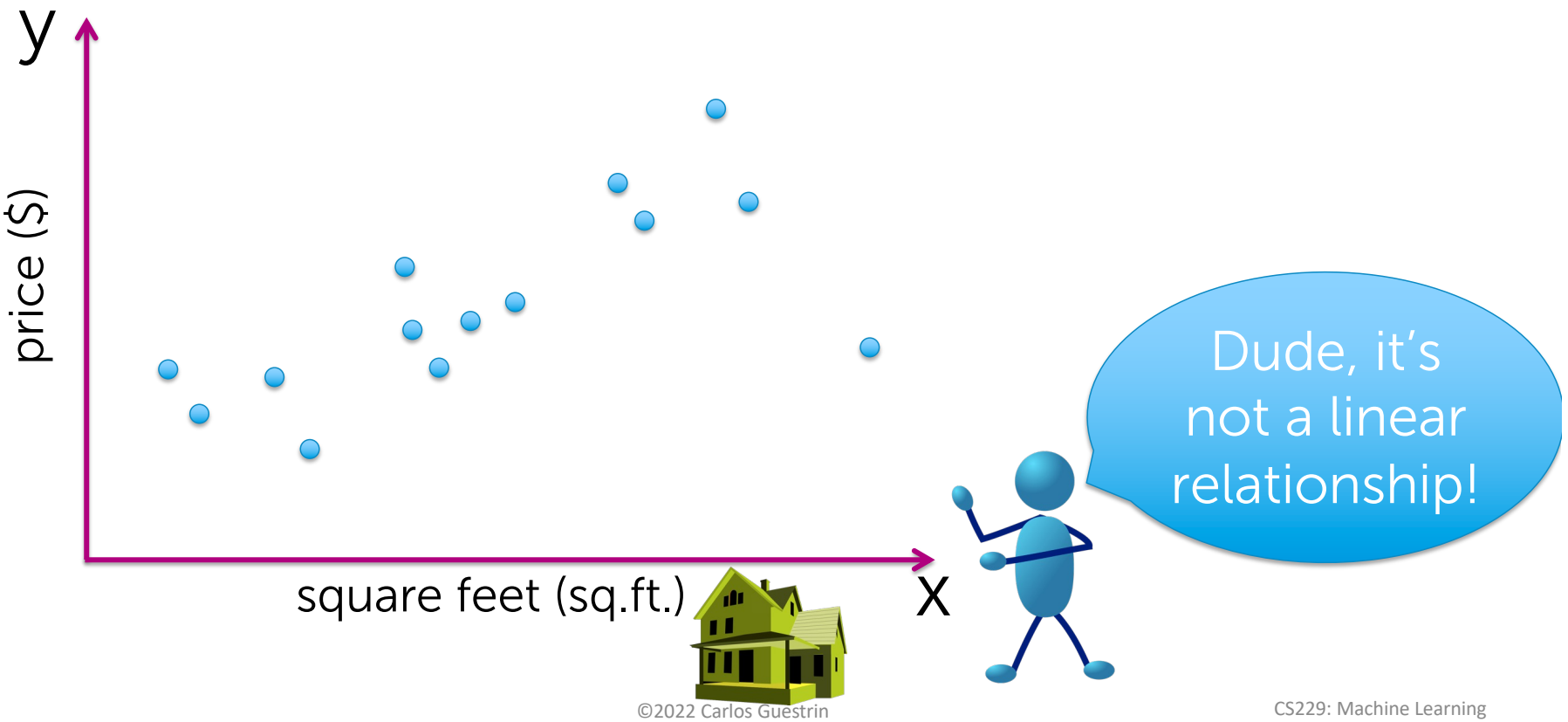
Bias-Variance Tradeoff

CS229: Machine Learning

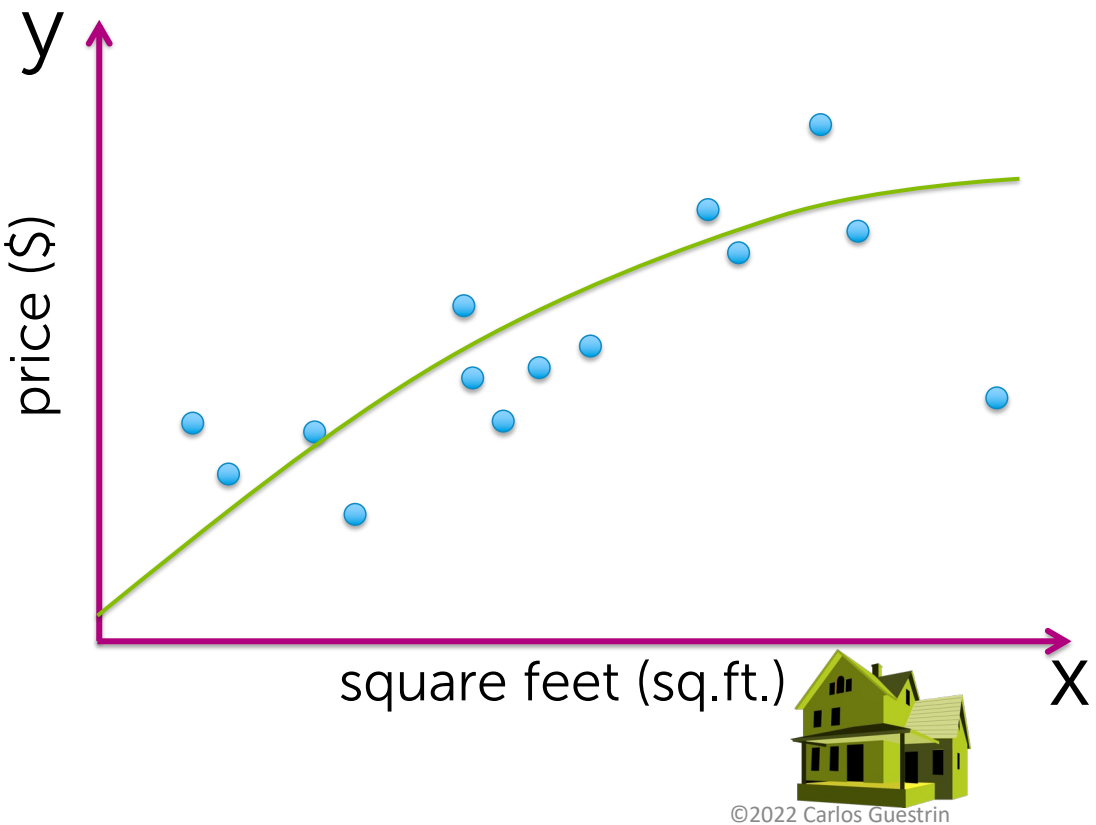
Carlos Guestrin
Stanford University

Slides include content developed by and co-developed with Emily Fox

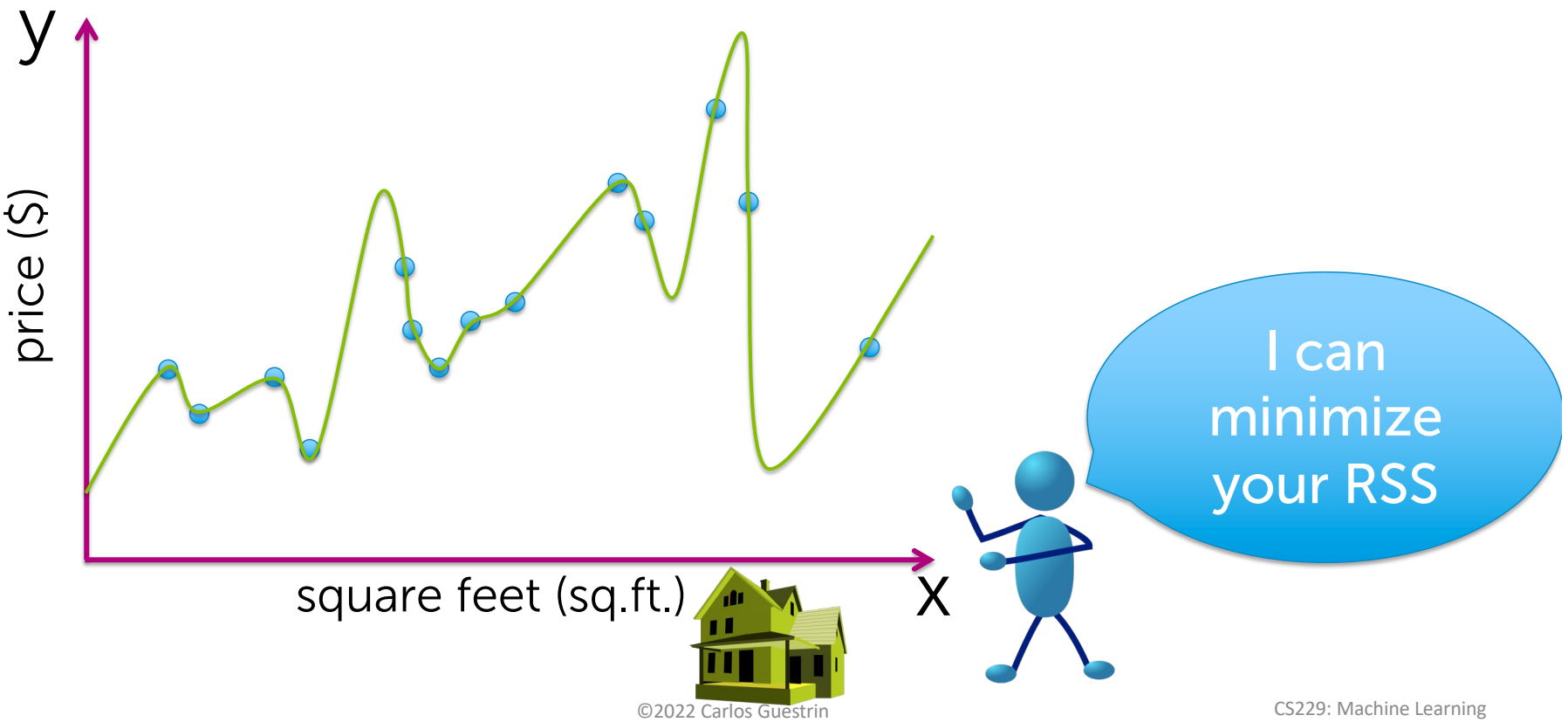
Fit data with a line or … ?



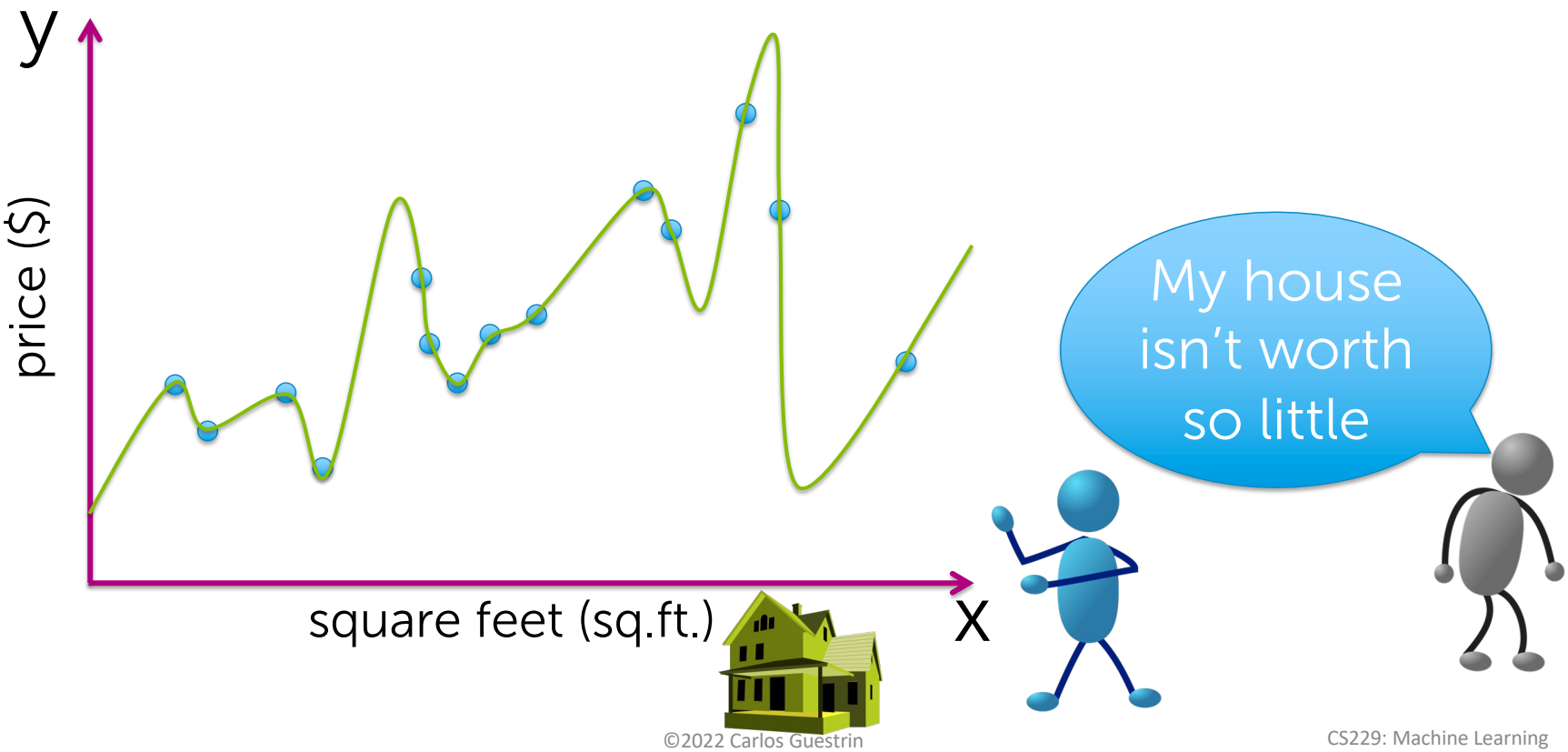
What about a quadratic function?



Even higher order polynomial



Do you believe this fit?



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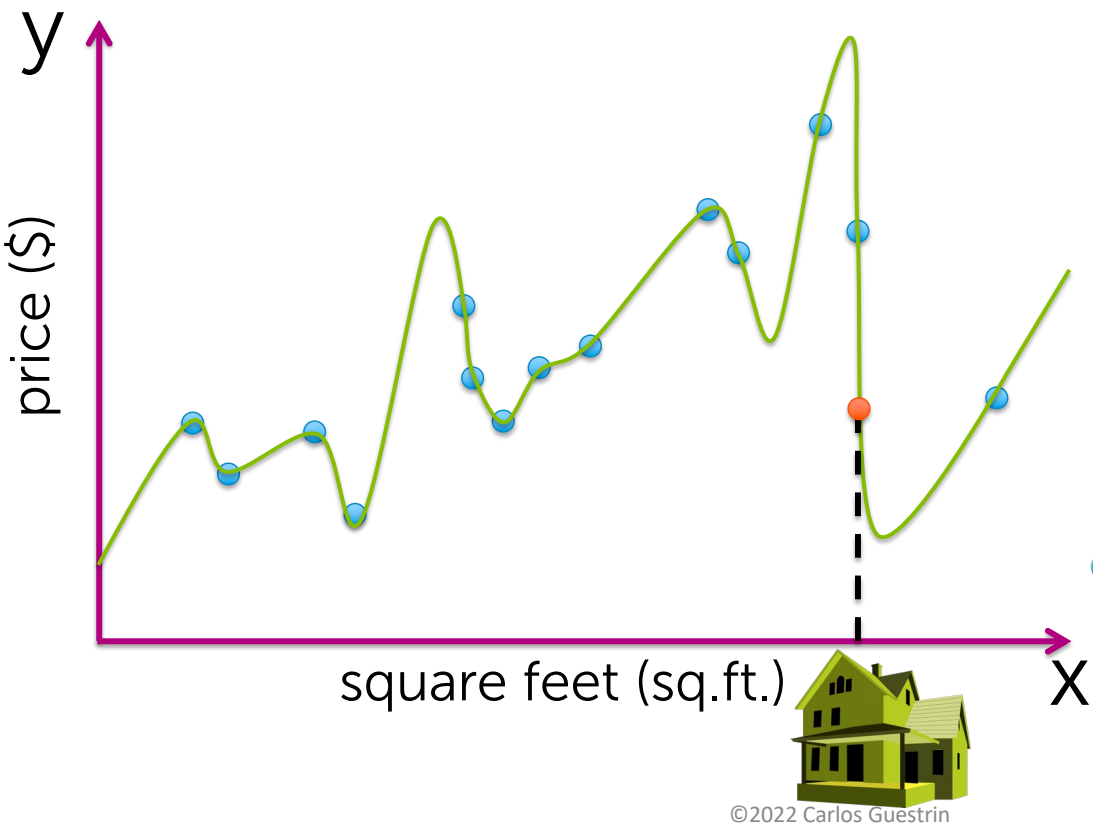
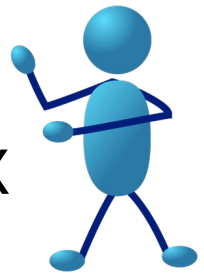
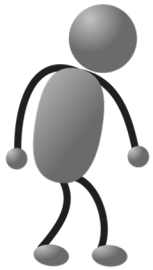


Minimizes RSS,
but bad predictions



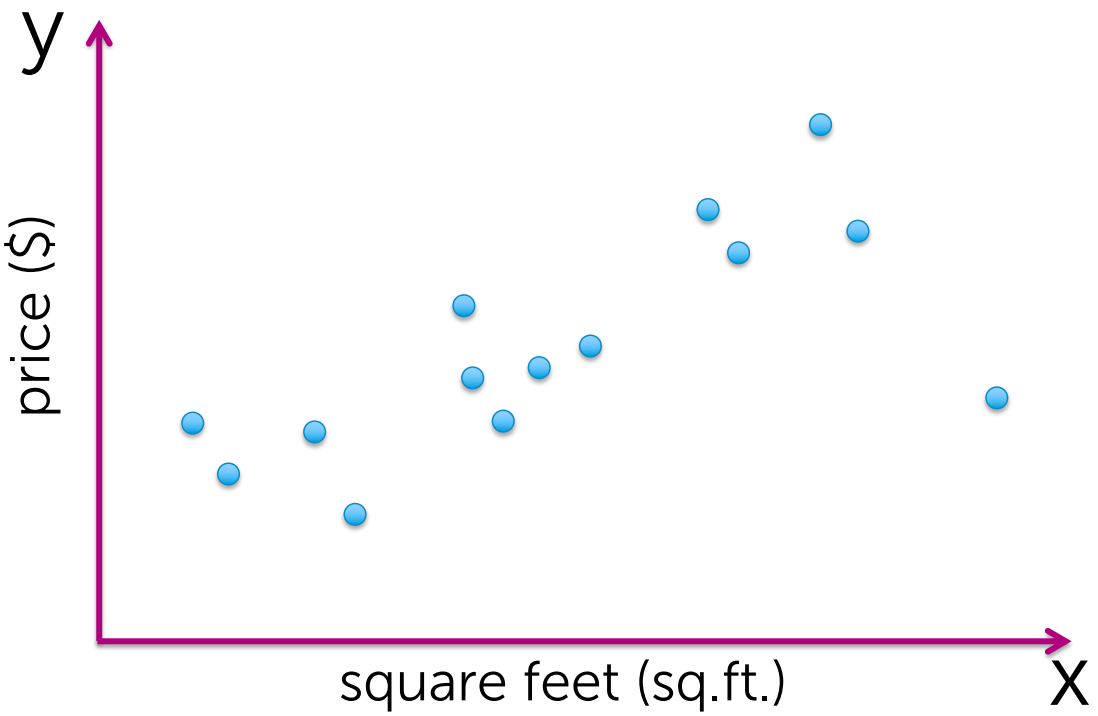


"Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful." George Box, 1987.

Assessing the loss

Assessing the loss
Part 1: Training error

Define training data



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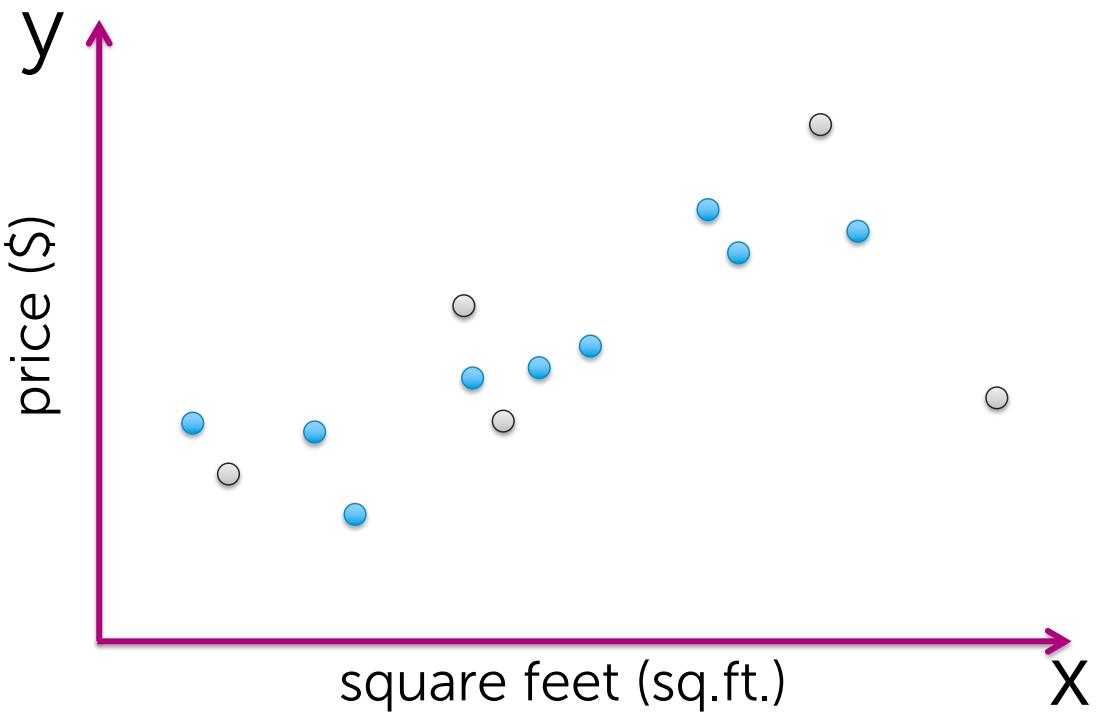
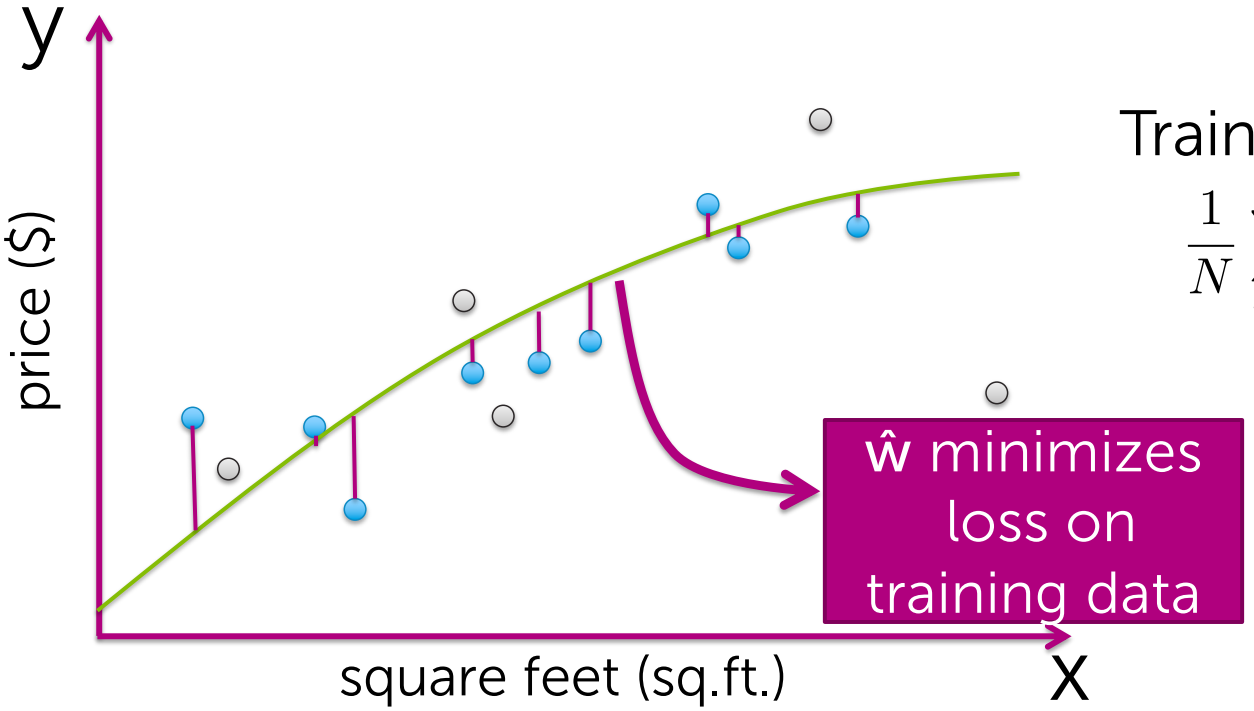
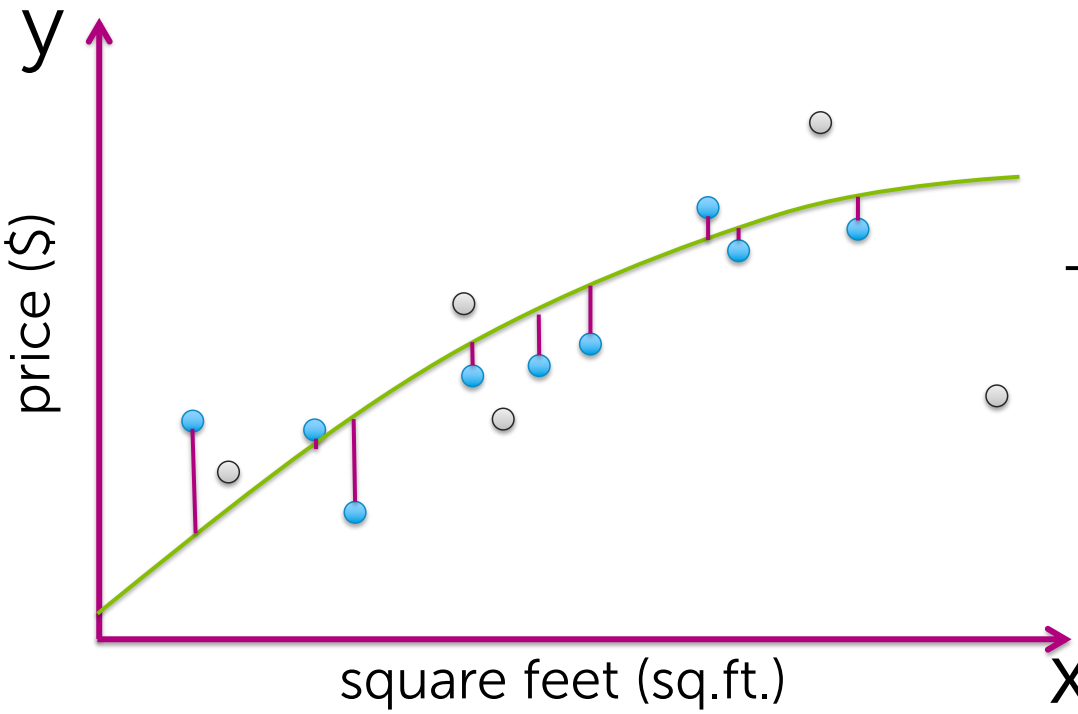


Example:
Fit quadratic to minimize RSS



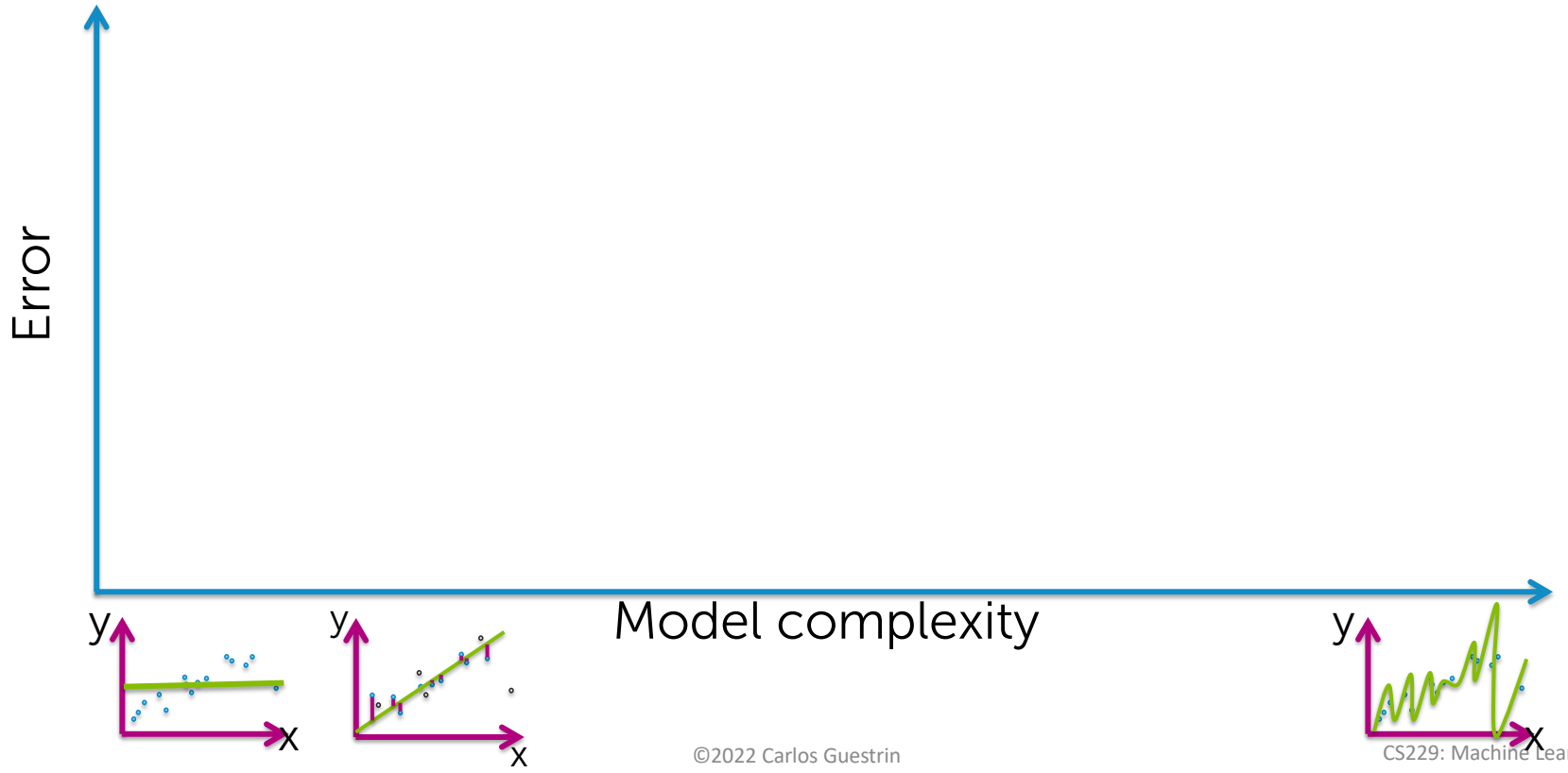
Training error ($\hat{w}$) = $\frac{1}{N}\sum_{i=1}^{N}(y_i - f_{\hat{w}}(x_i))^2$

Example:
Use squared error loss $(y-f_{\hat{w}}(x))^2$



Training error ($\hat{w}$) = 1/N *
[($\$_{train\ 1}$-$f_{\hat{w}}$(sq.ft.$_{train\ 1}$))^2
+ ($\$_{train\ 2}$-$f_{\hat{w}}$(sq.ft.$_{train\ 2}$))^2
+ ($\$_{train\ 3}$-$f_{\hat{w}}$(sq.ft.$_{train\ 3}$))^2
+ … include all training houses]

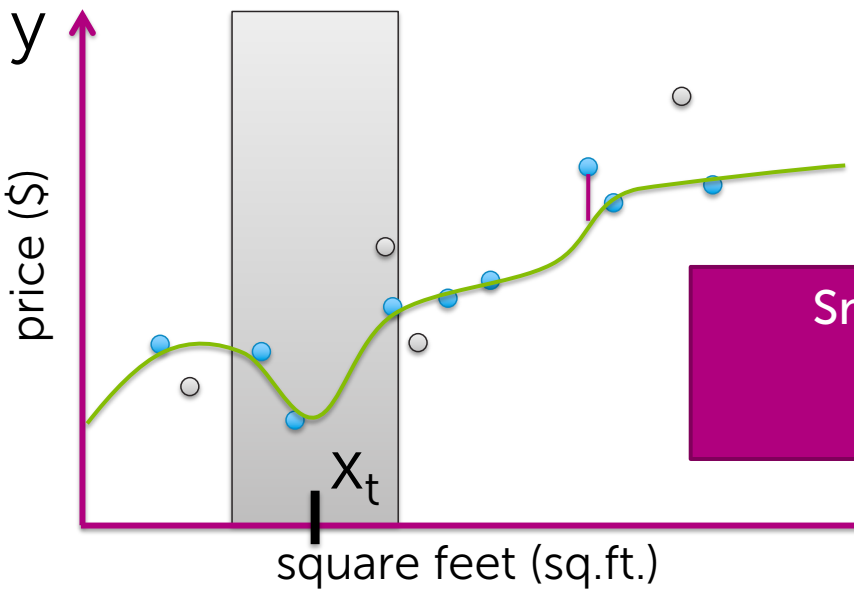
Training error vs. model complexity



Is training error a good measure of predictive performance?

Issue:

Training error is overly optimistic…$\hat{w}$ was fit to training data

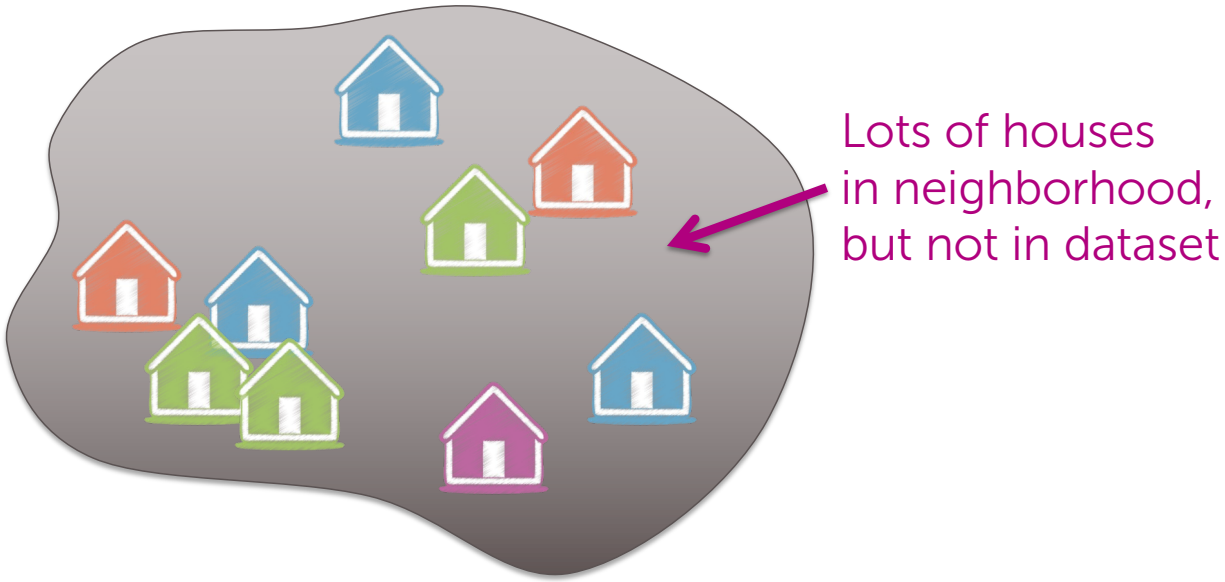


Small training error ≠ good predictions
(unless training data includes everything you might ever see)

Assessing the loss
Part 2: Generalization (true) error

Generalization error

Really want estimate of loss over all possible (,$) pairs



Generalization error definition

Really want estimate of loss over all possible ( ,$) pairs

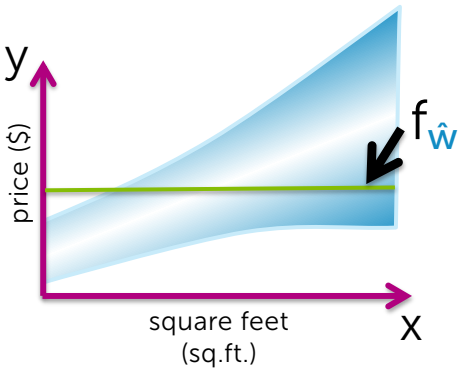
Formally:

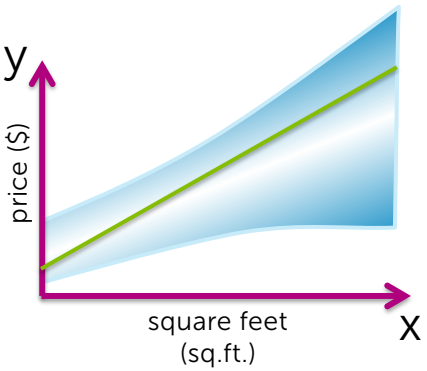
average over all possible (**x**,y) pairs weighted by how likely each is

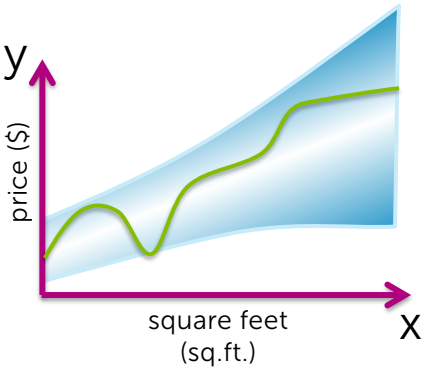
$$\text{generalization error} = E_{\mathbf{x},y}[L(y, f_{\hat{\mathbf{w}}}(\mathbf{x}))]$$

fit using training data

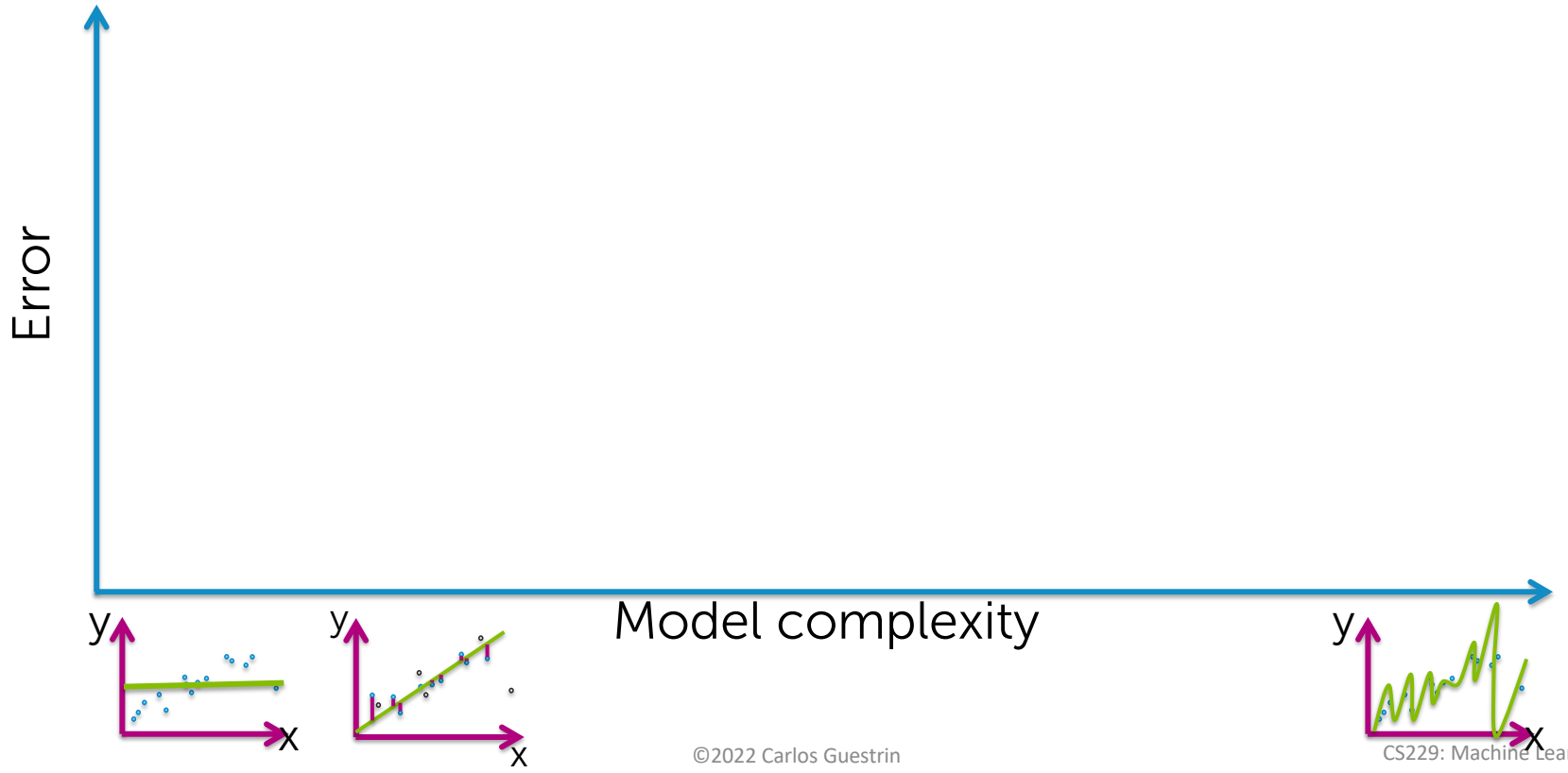
Generalization error vs. model complexity







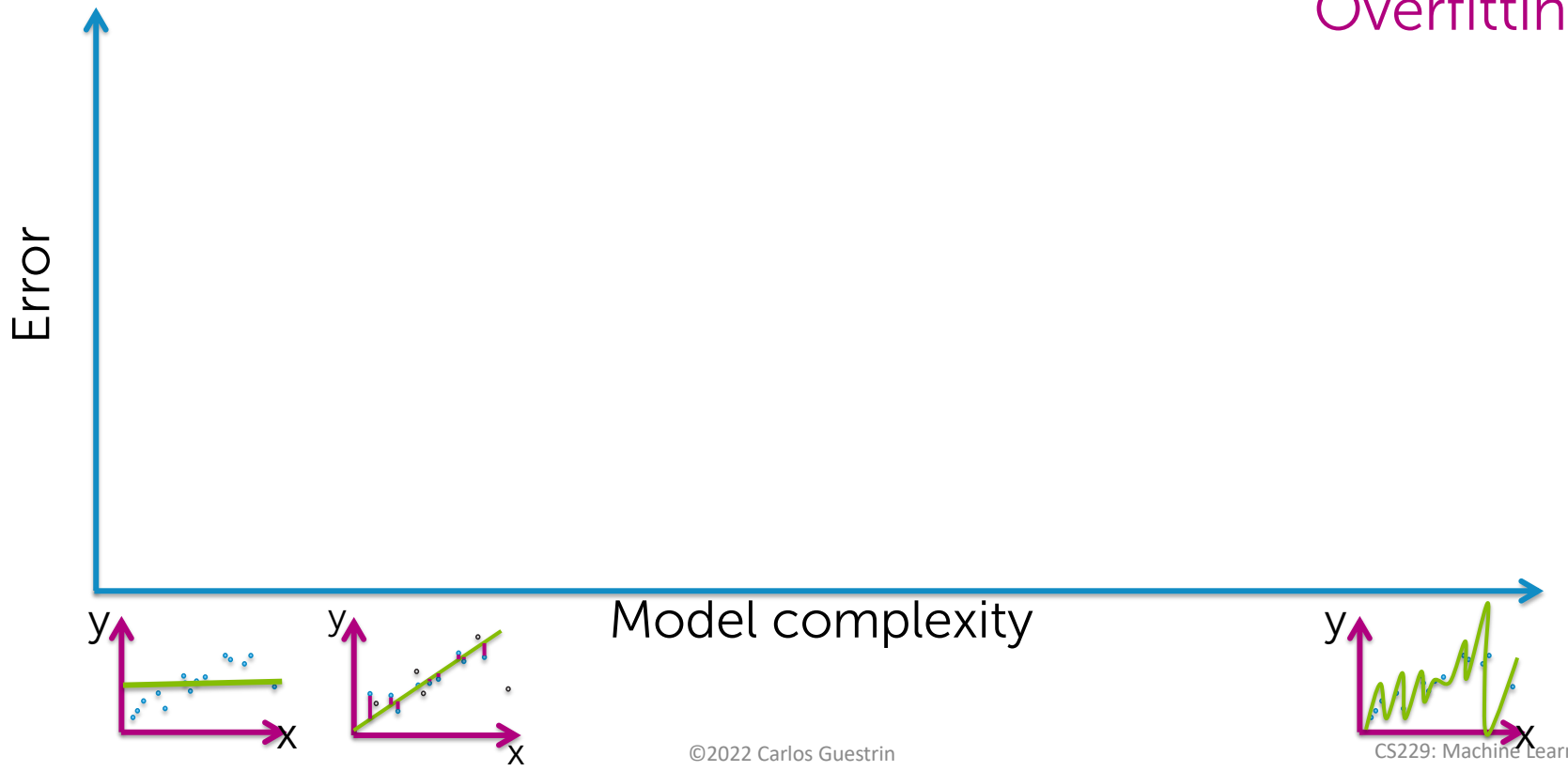
True error vs. model complexity



Assessing the loss
Part 3: Test error

Training, true, test error vs. model complexity

Overfitting if:



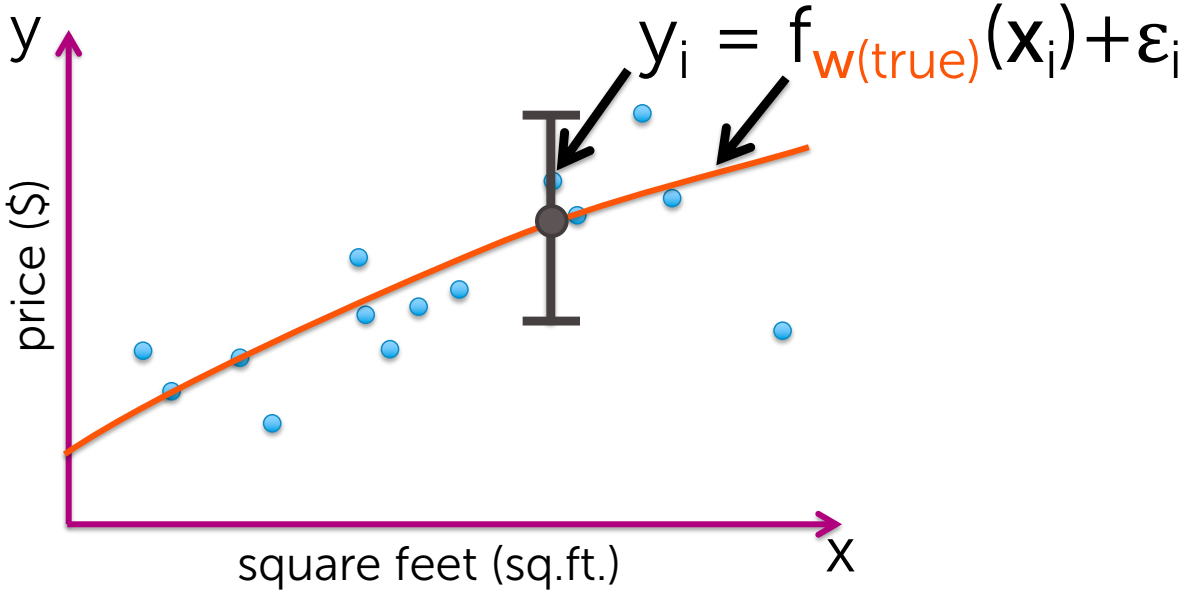
3 sources of error + the bias-variance tradeoff

3 sources of error

In forming predictions, there are 3 sources of error:

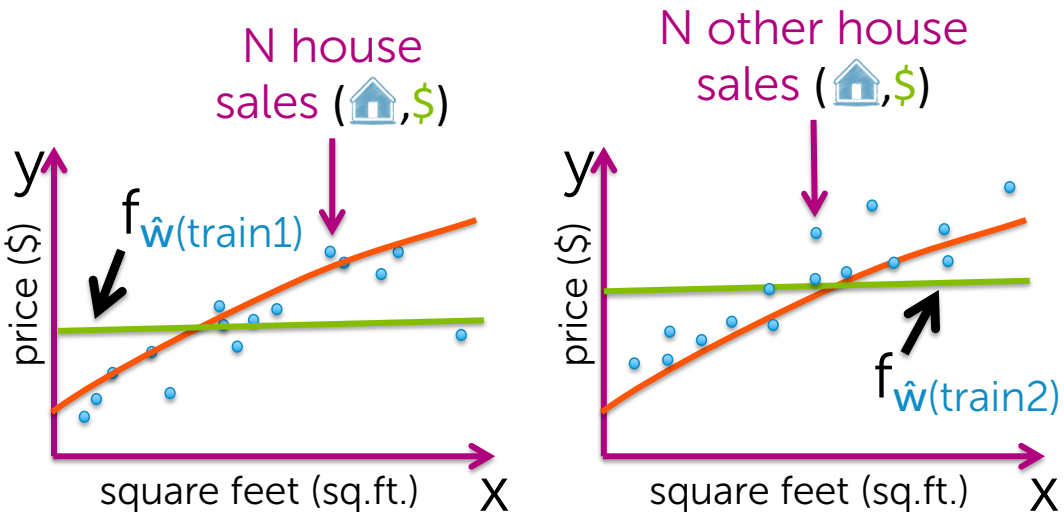
1. Noise
2. Bias
3. Variance

Data inherently noisy



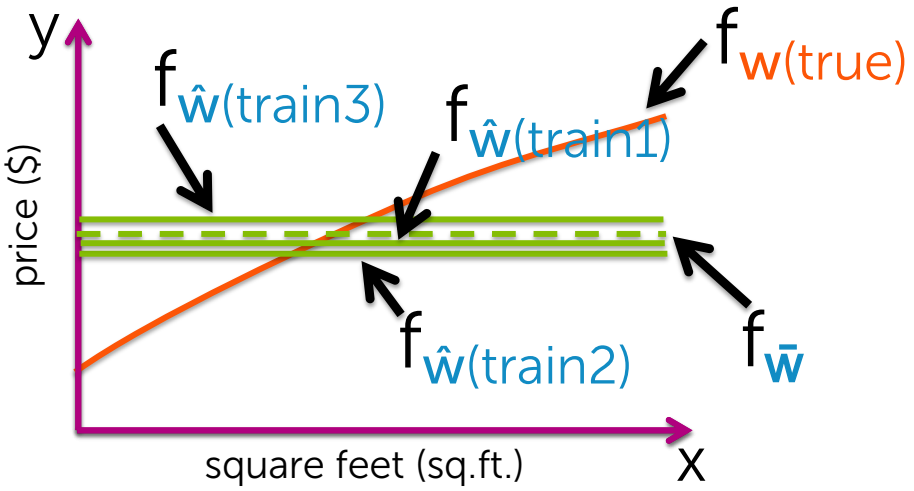
Bias contribution

Suppose we fit a constant function



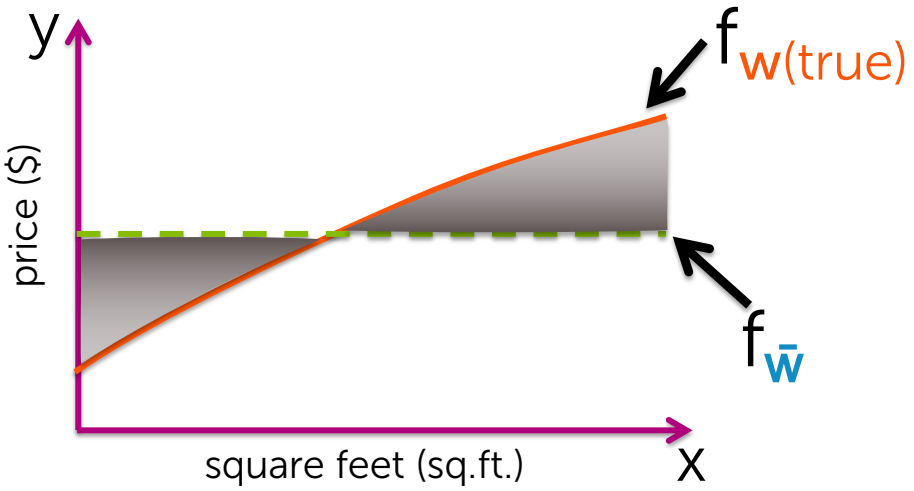
Bias contribution

Over all possible size N training sets, what do I expect my fit to be?



Bias contribution

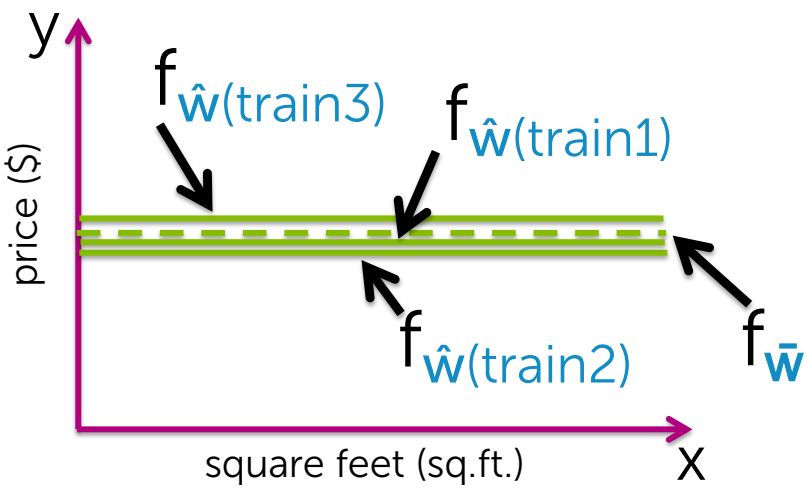
$\text{Bias}(\mathbf{x}) = f_{\mathbf{w}(\text{true})}(\mathbf{x}) - f_{\bar{\mathbf{w}}}(\mathbf{x})$ ← Is our approach flexible enough to capture $f_{\mathbf{w}(\text{true})}$? **If not, error in predictions.**



low complexity →

Variance contribution

How much do specific fits vary from the expected fit?



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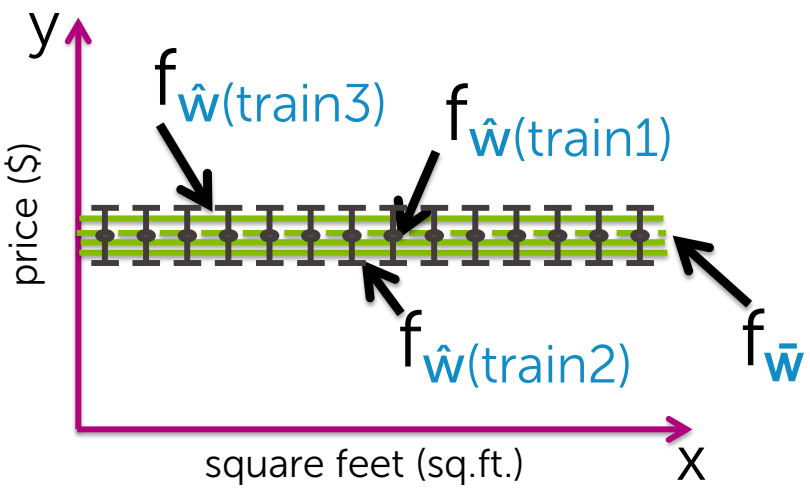

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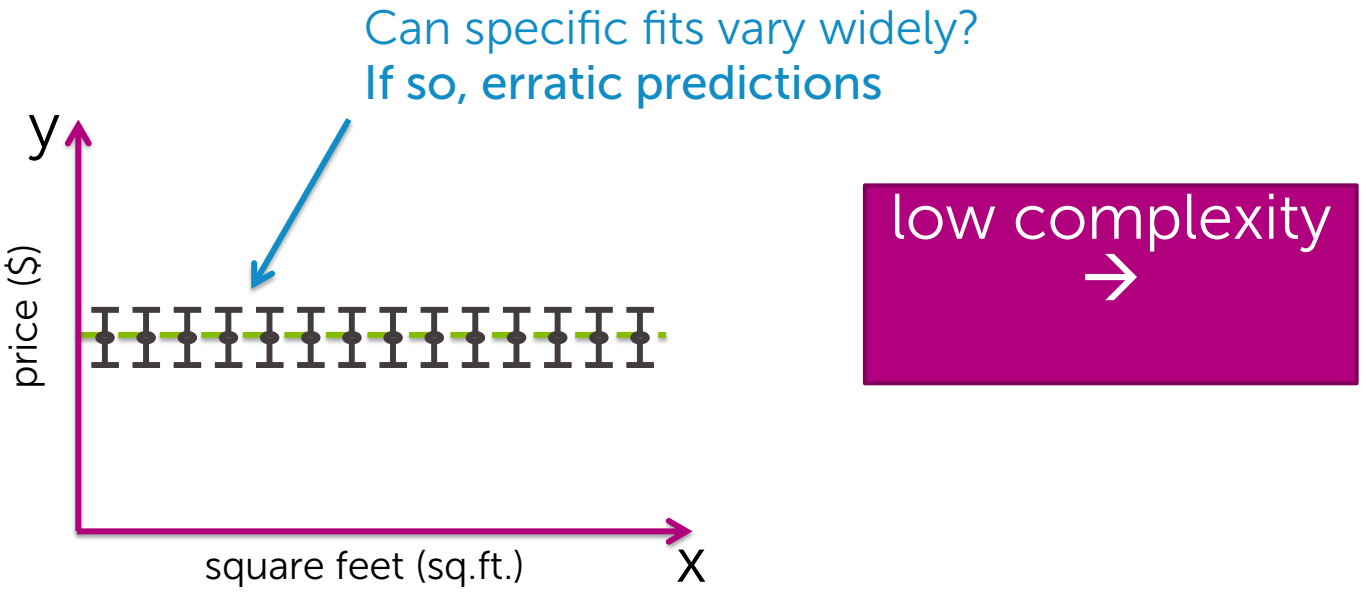
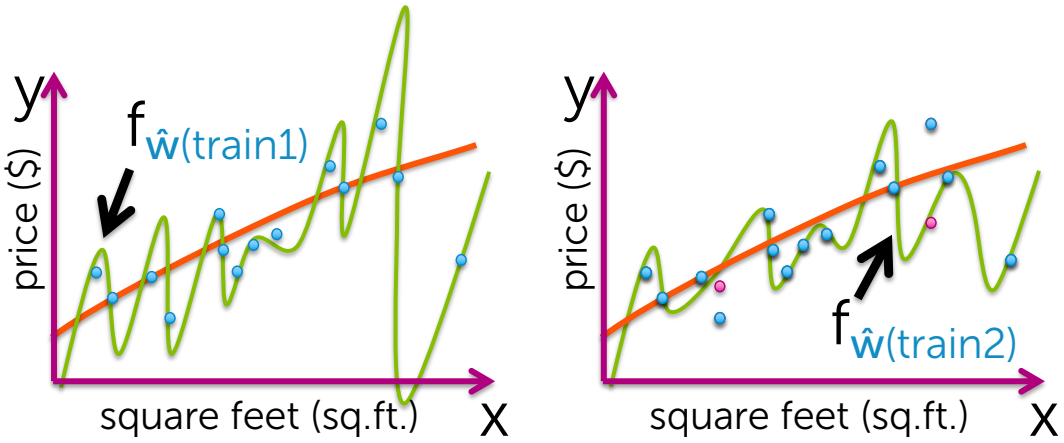


Variance of high-complexity models

Assume we fit a high-order polynomial



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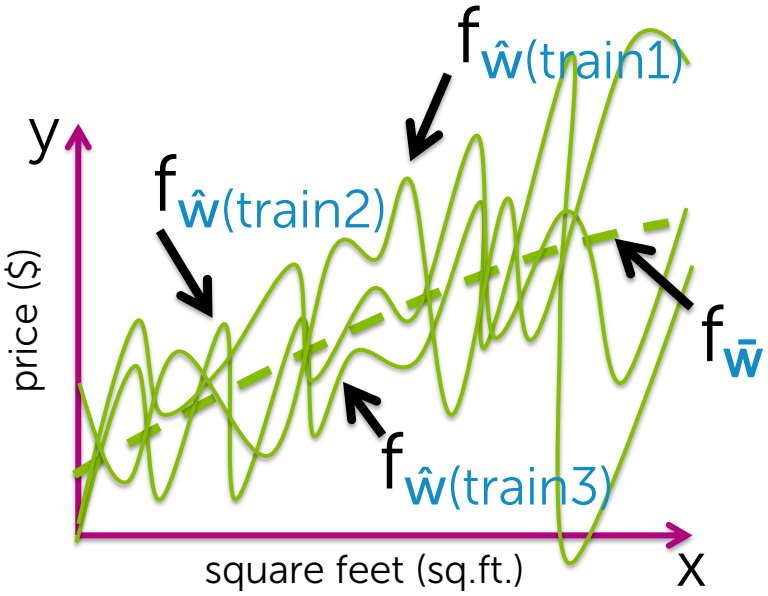
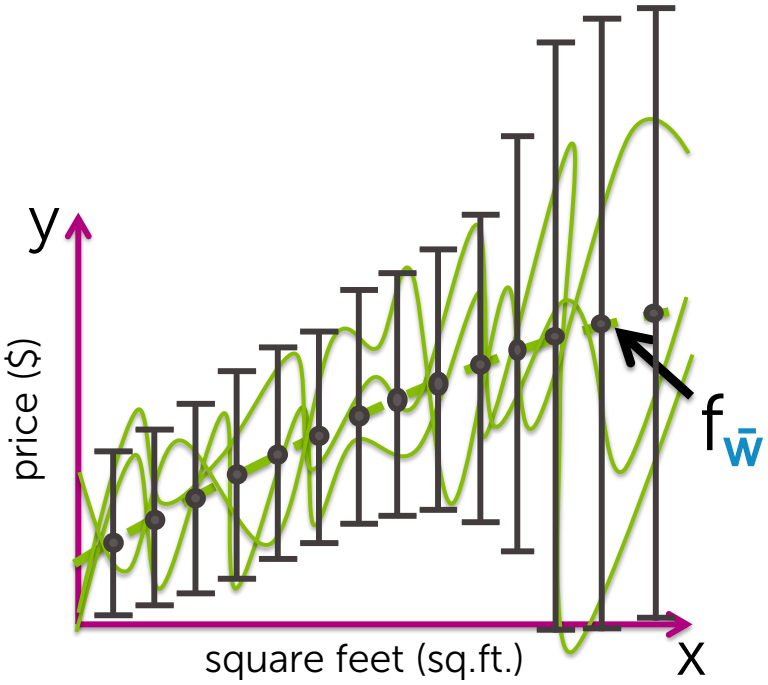
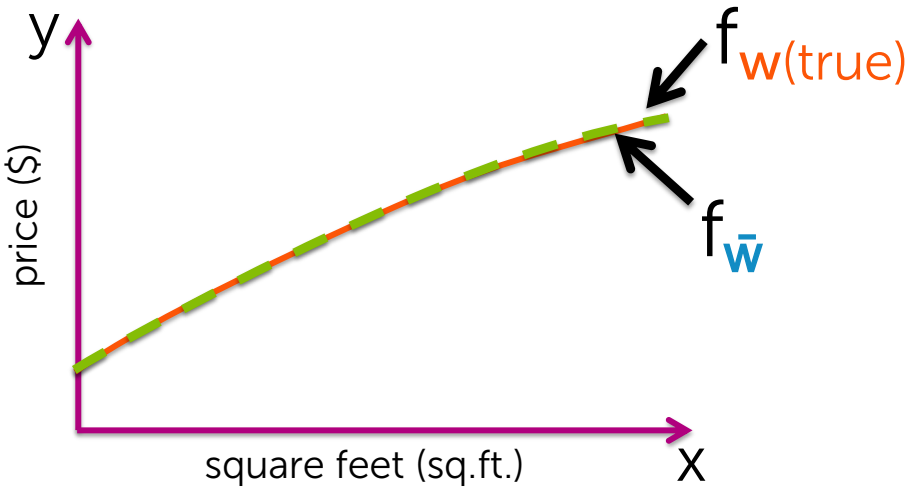


Variance of high-complexity models



high complexity
→

Bias of high-complexity models

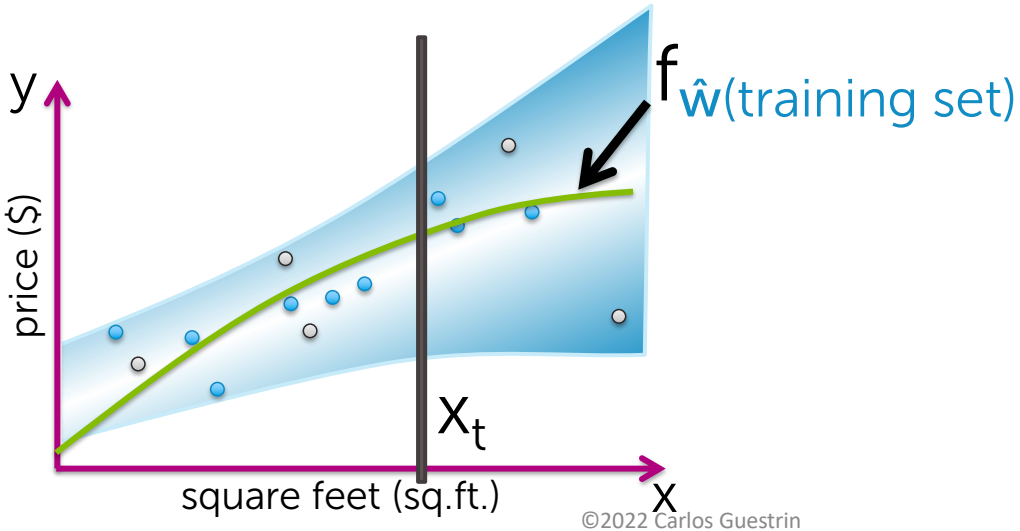


high complexity
→

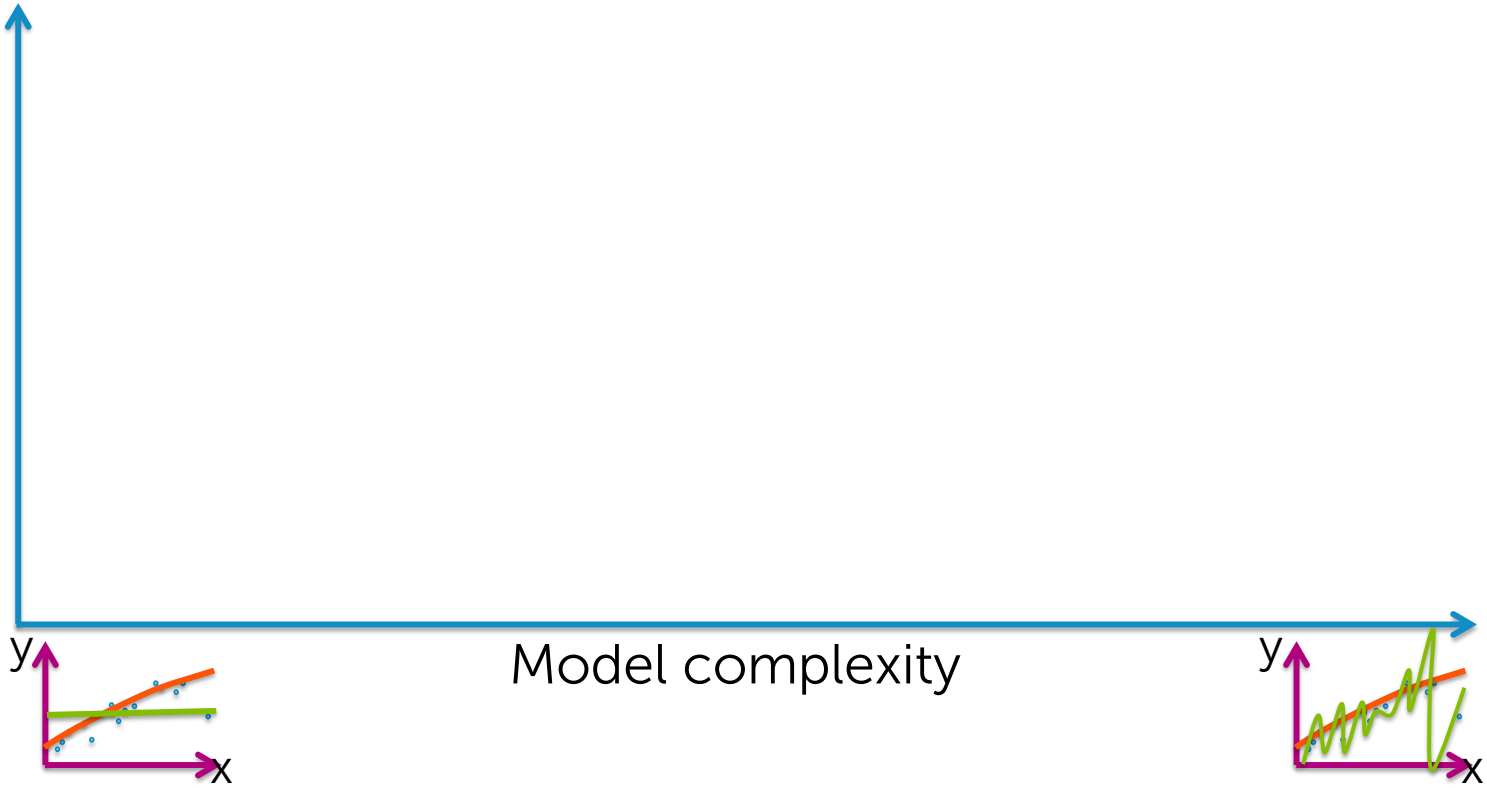
Sum of 3 sources of error

Average squared error at x_t

$$= \sigma^2 + [\text{bias}(f_{\hat{w}}(x_t))]^2 + \text{var}(f_{\hat{w}}(x_t))$$



Bias-variance tradeoff



Error vs. amount of data

Why 3 sources of error?
A formal derivation

Deriving expected prediction error

Expected prediction error

$= E_{train}$ [generalization error of $\hat{\mathbf{w}}(train)$]

$= E_{train}\left[E_{\mathbf{x},y}[L(y, f_{\hat{\mathbf{w}}(train)}(\mathbf{x}))]\right]$

1. Look at specific $\mathbf{x}_t$
2. Consider $L(y, f_{\hat{\mathbf{w}}}(\mathbf{x})) = (y - f_{\hat{\mathbf{w}}}(\mathbf{x}))^2$

Expected prediction error at $\mathbf{x}_t$

$= E_{train, y_t}\left[(y_t - f_{\hat{\mathbf{w}}(train)}(\mathbf{x}_t))^2\right]$

Simplifying Notation

- Expected prediction error at $\mathbf{x}_t$

  $= E_{train,y_t}\left[(y_t - f_{\hat{\mathbf{w}}(train)}(\mathbf{x}_t))^2\right]$

- Simple (and abusive ☺) notation:
  - $y_t \rightarrow y$
  - $f_{\mathbf{w}(true)}(\mathbf{x}_t) \rightarrow f$
  - $f_{\hat{\mathbf{w}}(train)}(\mathbf{x}_t) \rightarrow \hat{f}$
  - $E_{train}\left[f_{\hat{\mathbf{w}}(train)}(\mathbf{x}_t)\right] = f_{\bar{w}}(\mathbf{x}_t) \rightarrow \bar{f}$

Deriving expected prediction error

Expected prediction error at $\mathbf{x}_t$

$$= E_{train, y_t}\left[(y_t - f_{\hat{\mathbf{w}}(train)}(\mathbf{x}_t))^2\right] = E_{train}\left[(y - \hat{f})^2\right] =$$

$$= E_{train}\left[(y - f) + (f - \hat{f}))^2\right]$$

Equating MSE with bias and variance

$$\text{MSE}[f_{\hat{w}(\text{train})}(x_t)]$$

$$= E_{\text{train}}[(f - \hat{f})^2]$$

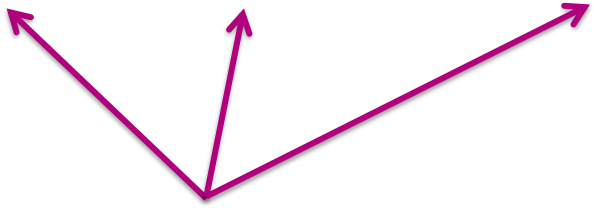
$$= E_{\text{train}}[((f - \bar{f}) + (\bar{f} - \hat{f}))^2]$$

Putting it all together

Expected prediction error at $\mathbf{x}_t$

$$= \sigma^2 + \text{MSE}\left[f_{\hat{\mathbf{w}}}(\mathbf{x}_t)\right]$$

$$= \sigma^2 + \left[\text{bias}(f_{\hat{\mathbf{w}}}(\mathbf{x}_t))\right]^2 + \text{var}(f_{\hat{\mathbf{w}}}(\mathbf{x}_t))$$



3 sources of error

Summary of bias-variance tradeoff

What you can do now…

- Contrast relationship between model complexity and train, true and test loss
- Compute training and test error given a loss function for different model complexities
- List and interpret the 3 sources of avg. prediction error
  - Irreducible error, bias, and variance

Annotated bias Slides

Bias-Variance Tradeoff

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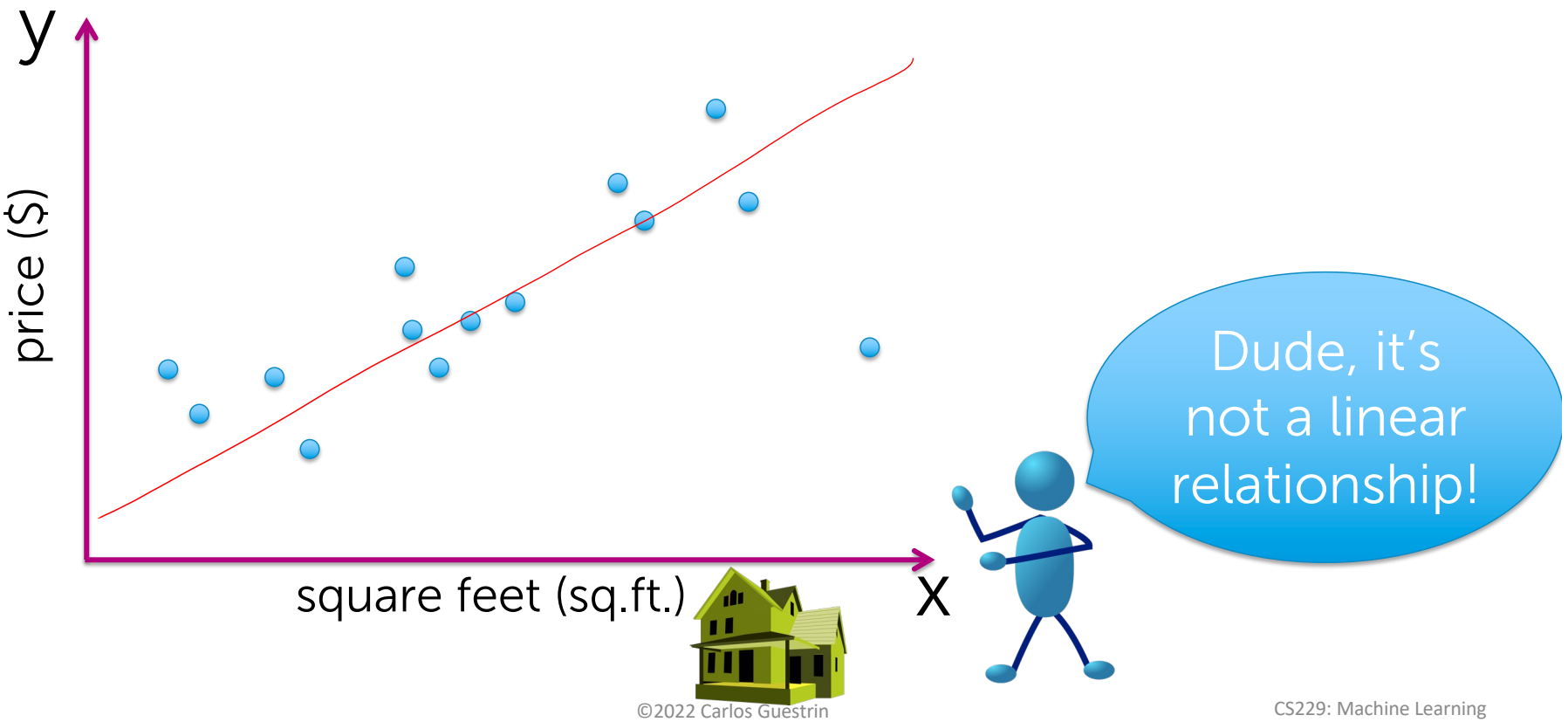
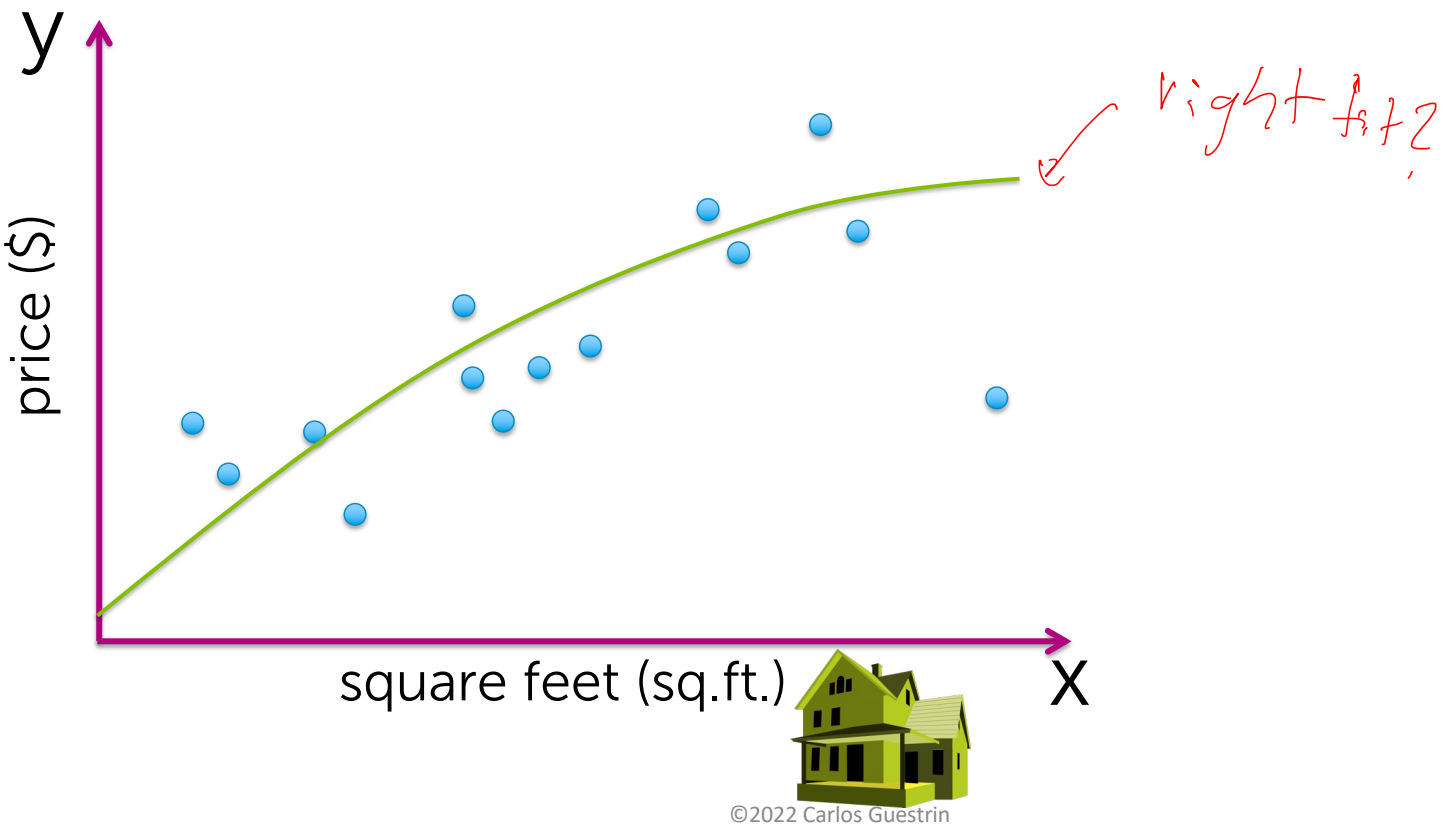
Slides include content developed by and co-developed with Emily Fox

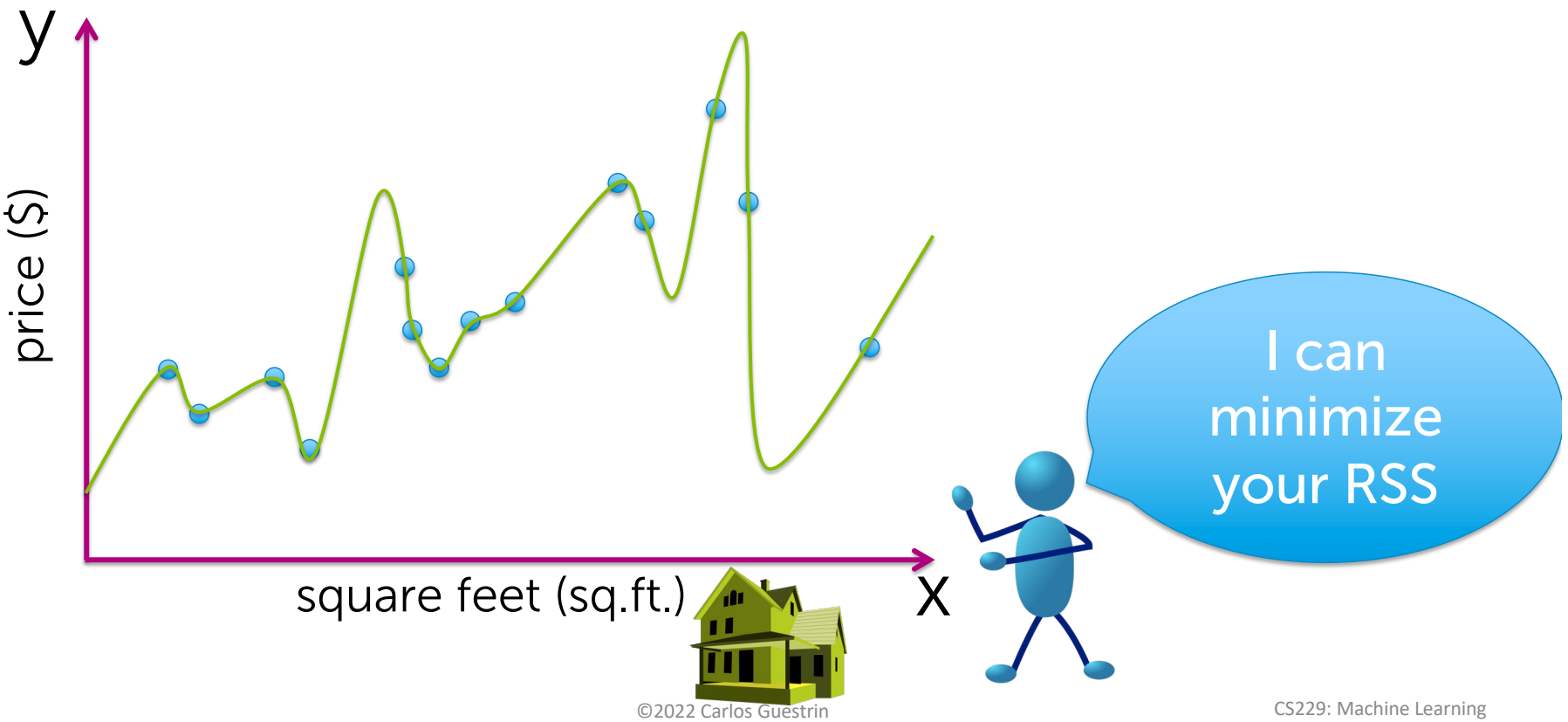
Fit data with a line or … ?



What about a quadratic function?



Even higher order polynomial



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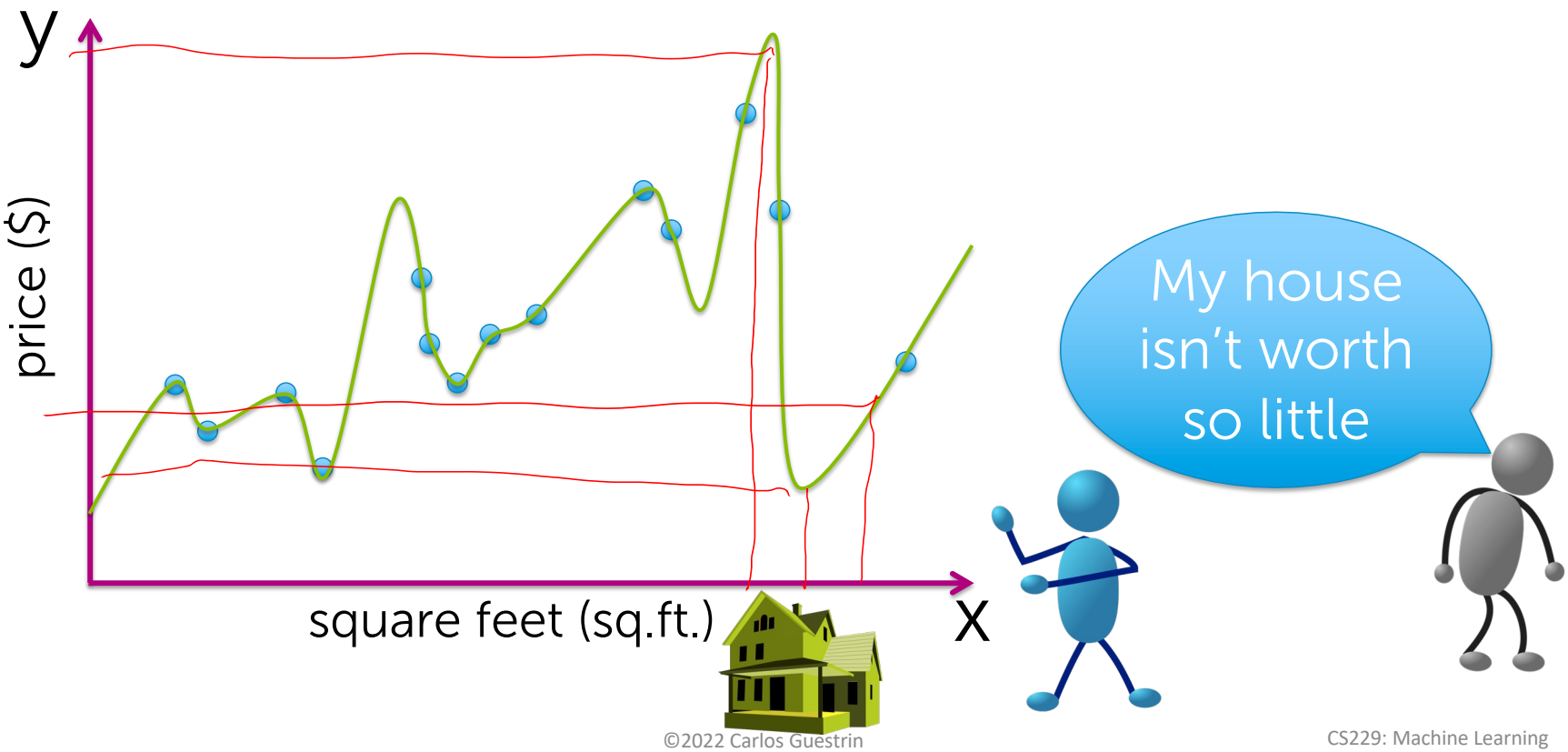

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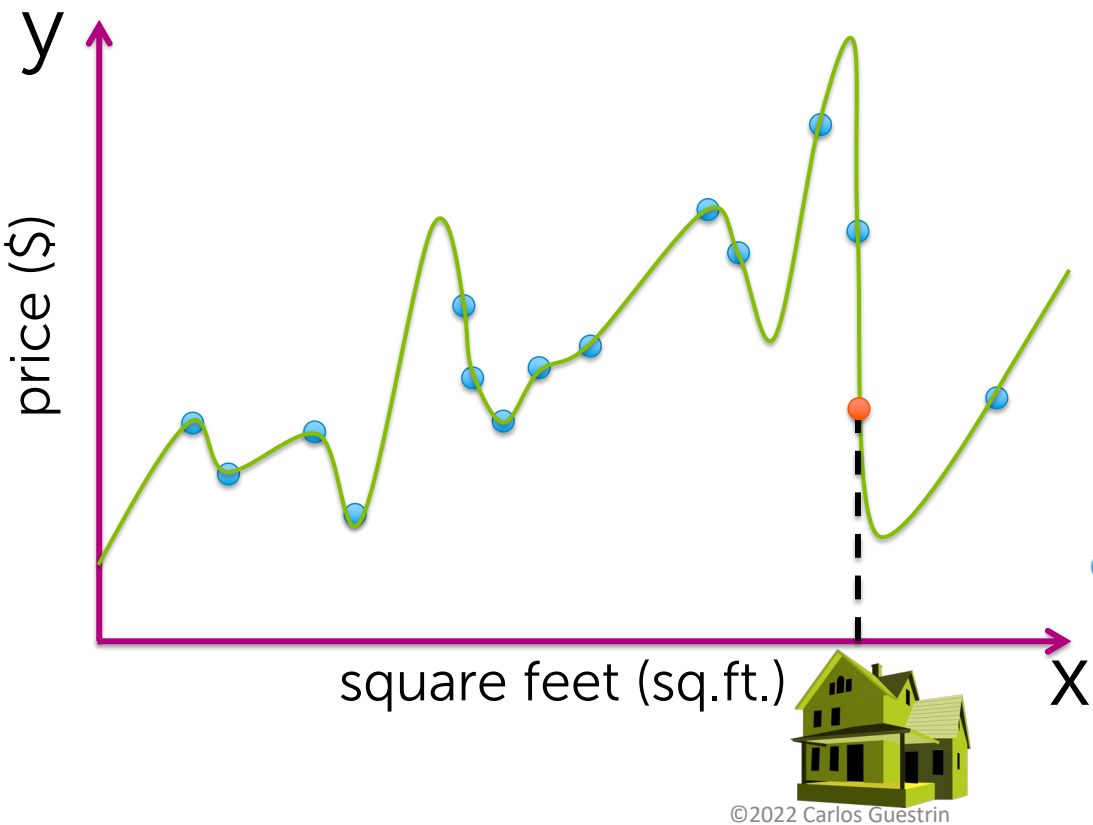
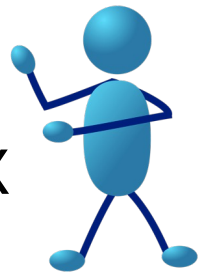
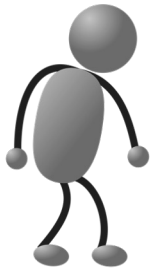


Minimizes RSS,
but bad predictions





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Assessing the loss

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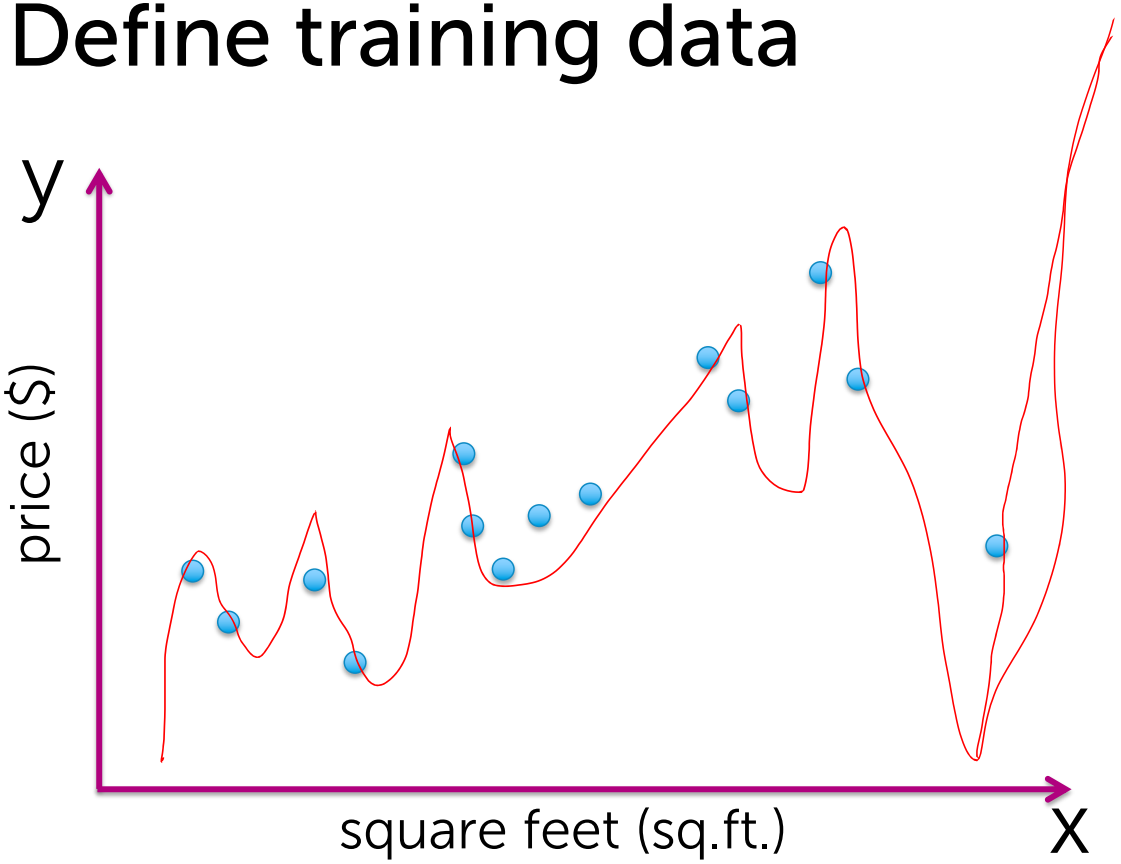

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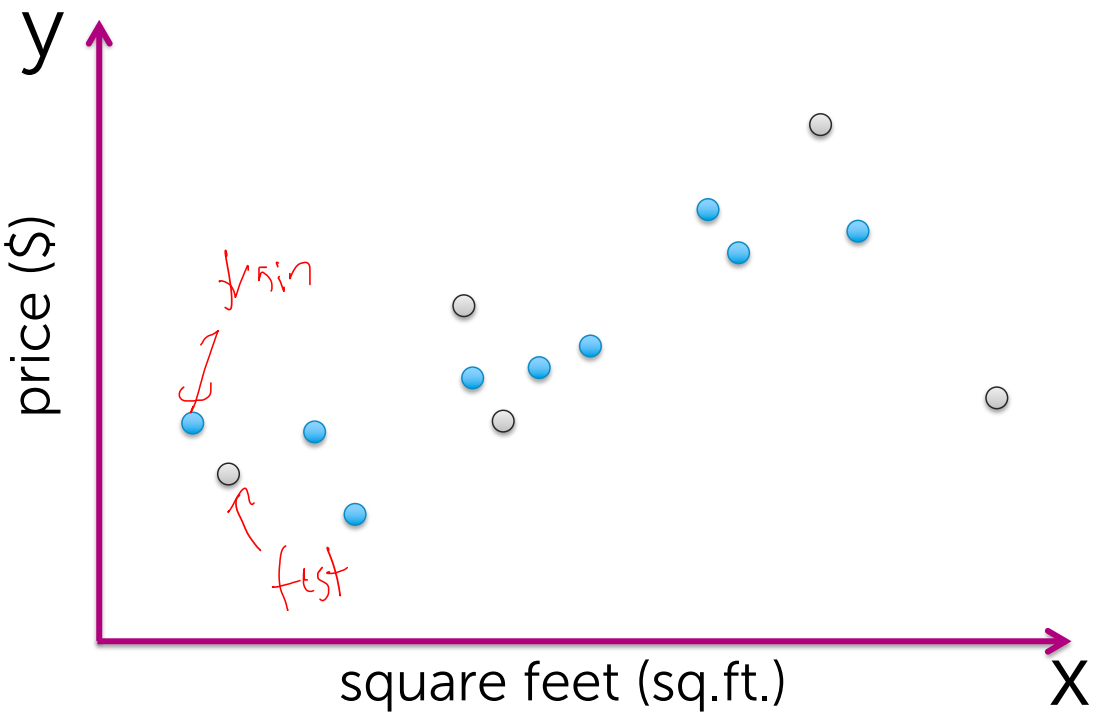
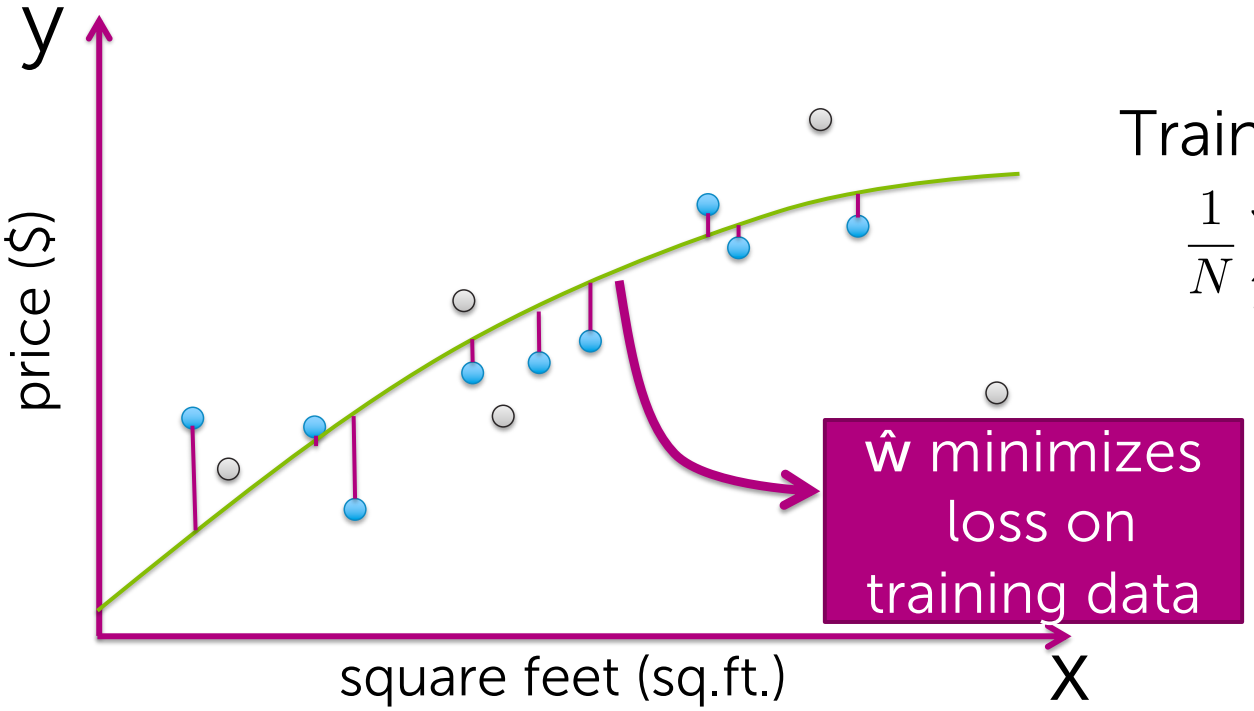


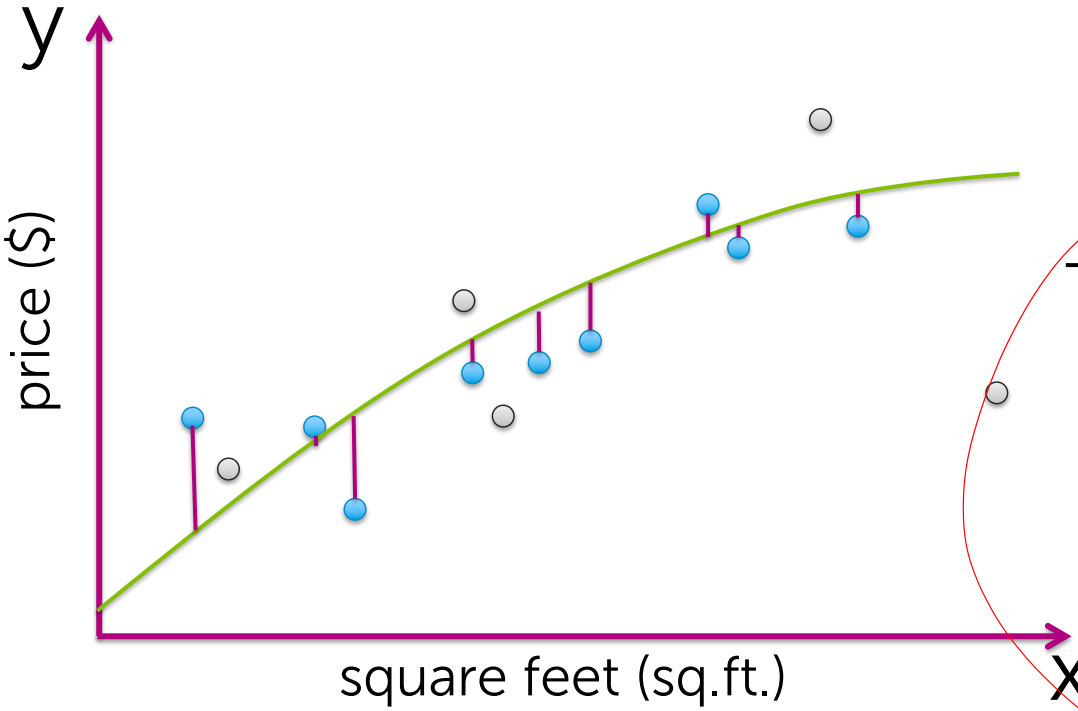
Example:
Fit quadratic to minimize RSS



Training error ($\hat{w}$) =

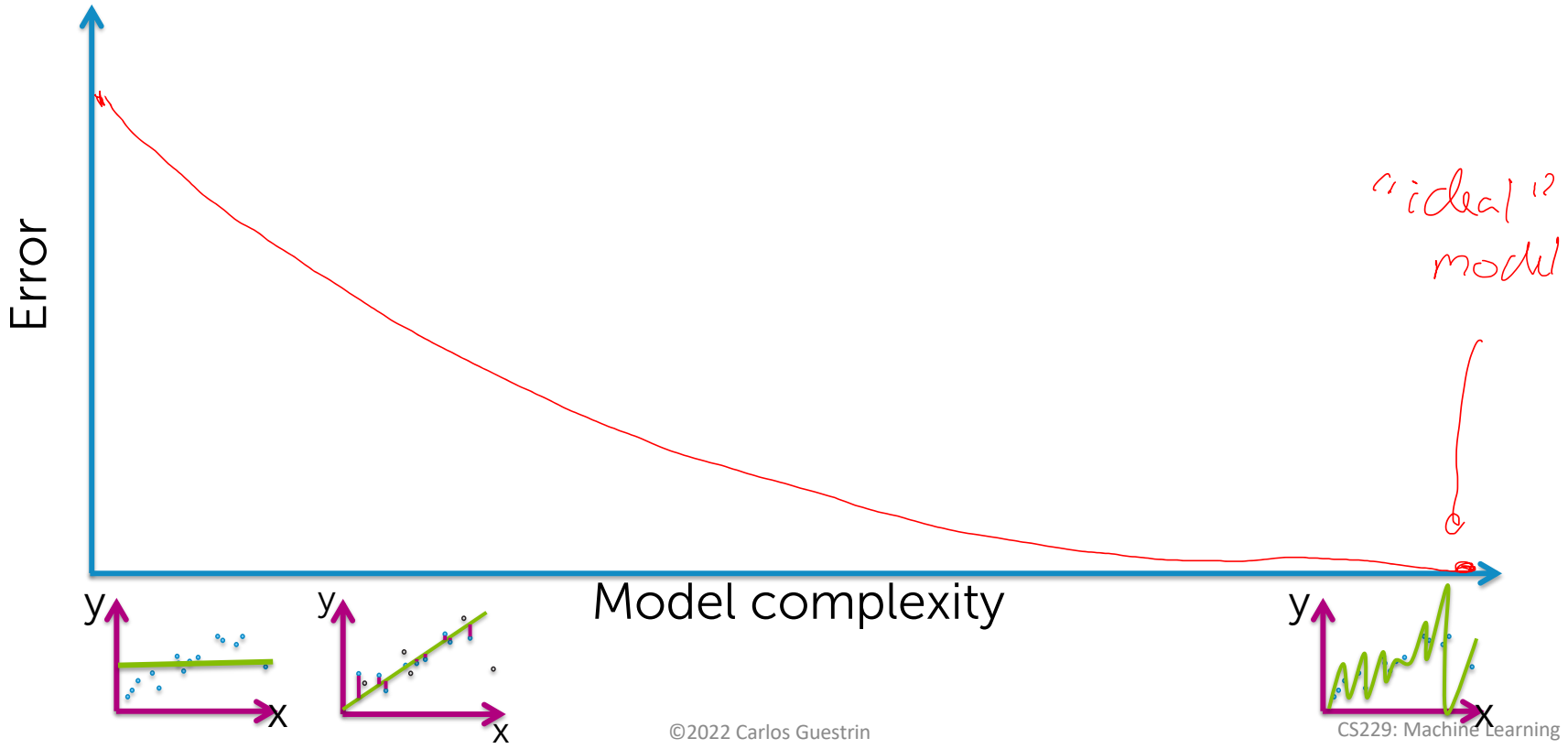
$$\frac{1}{N}\sum_{i=1}^{N}(y_i - f_{\hat{w}}(x_i))^2$$

Example:
Use squared error loss $(y-f_{\hat{w}}(x))^2$



Training error ($\hat{w}$) = 1/N *
[($\$_{train\ 1}$ - $f_{\hat{w}}(sq.ft._{train\ 1})$)^2
+ ($\$_{train\ 2}$ - $f_{\hat{w}}(sq.ft._{train\ 2})$)^2
+ ($\$_{train\ 3}$ - $f_{\hat{w}}(sq.ft._{train\ 3})$)^2
+ … include all training houses]

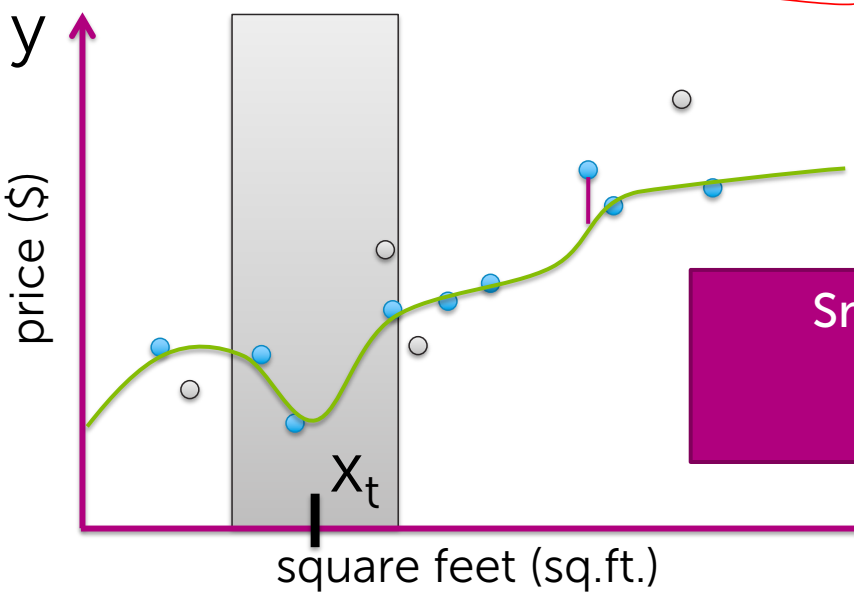
Training error vs. model complexity



Is training error a good measure of predictive performance?

Issue:

Training error is overly optimistic…$\hat{w}$ was fit to training data

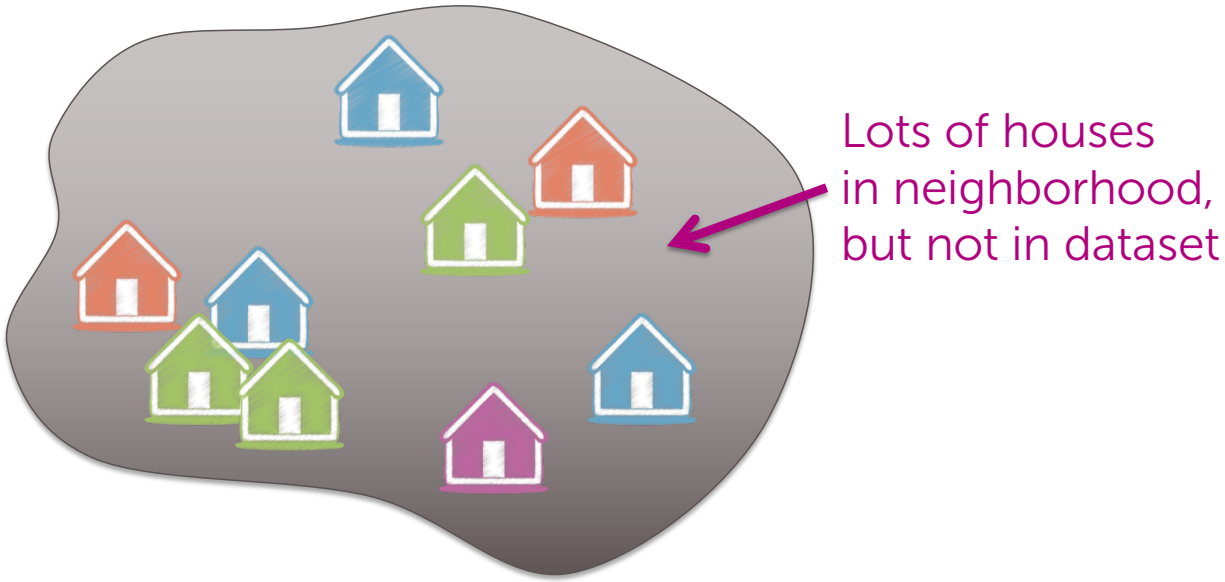


Small training error ≠ good predictions
(unless training data includes everything you might ever see)

Assessing the loss
Part 2: Generalization (true) error

Generalization error

Really want estimate of loss over all possible (,$) pairs



Generalization error definition

Really want estimate of loss over all possible (, $) pairs

Formally:

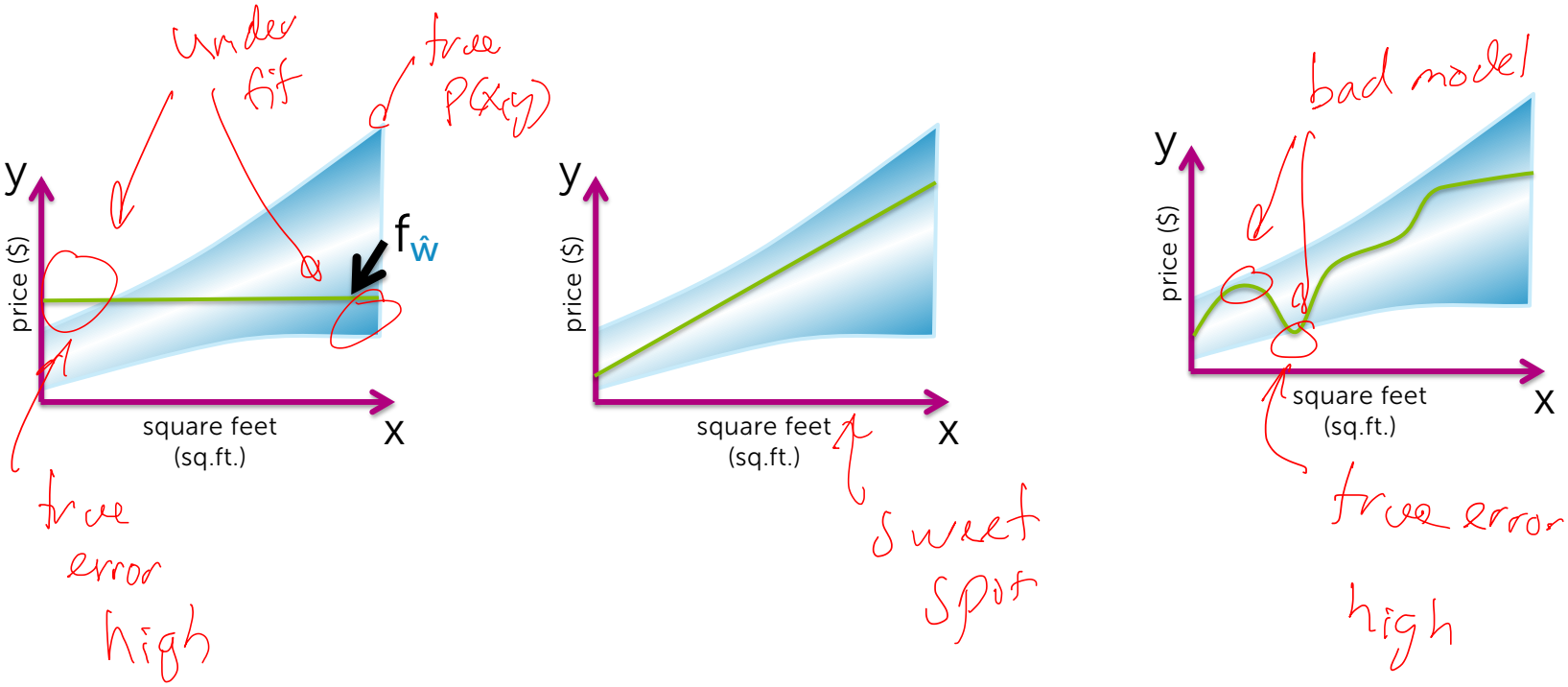
average over all possible (**x**,y) pairs weighted by how likely each is

$$\text{generalization error} = E_{\mathbf{x},y}[L(y, f_{\hat{\mathbf{w}}}(\mathbf{x}))]$$

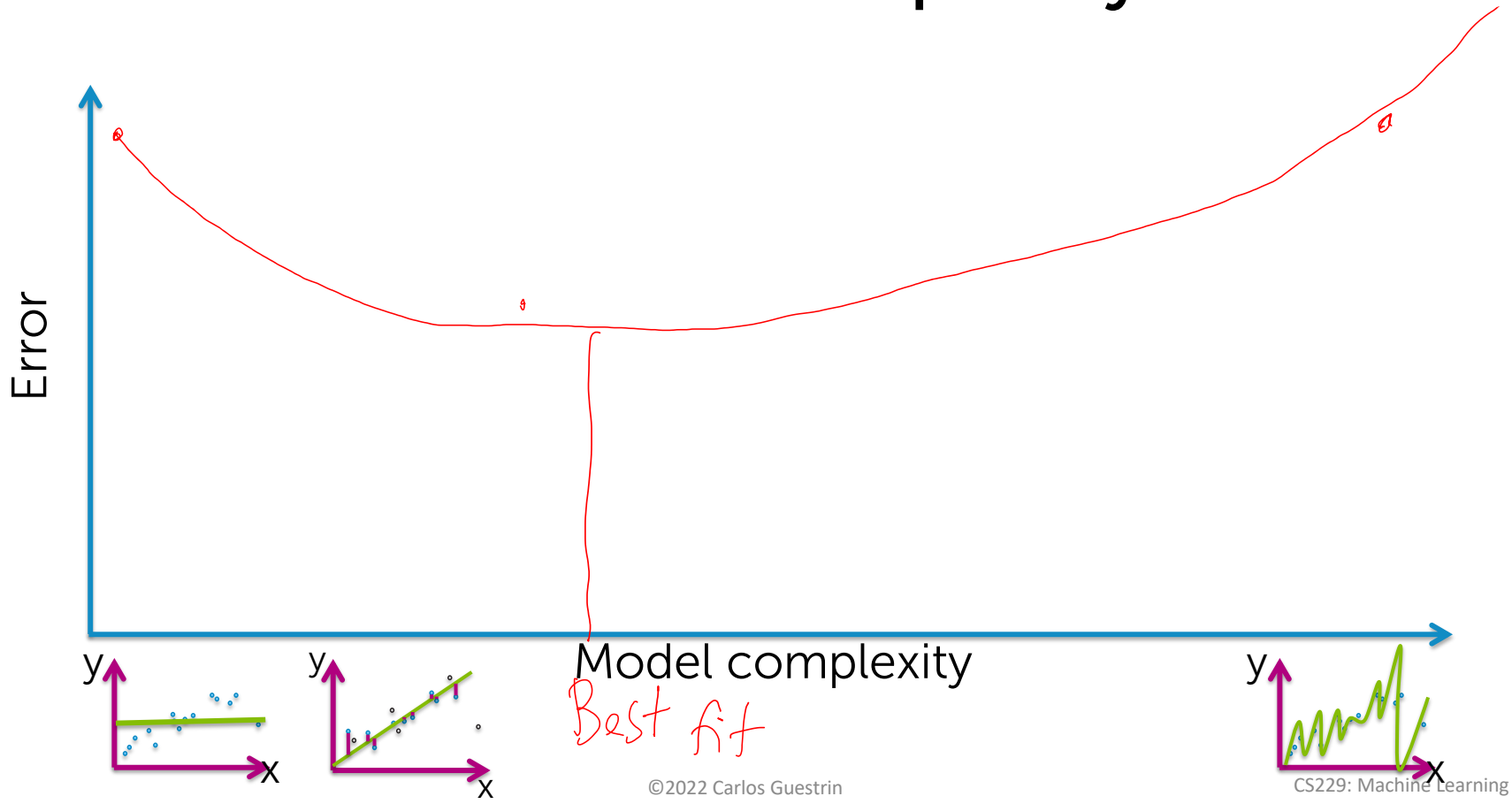
fit using training data

↳ true prob. $p(x,y)$

Generalization error vs. model complexity

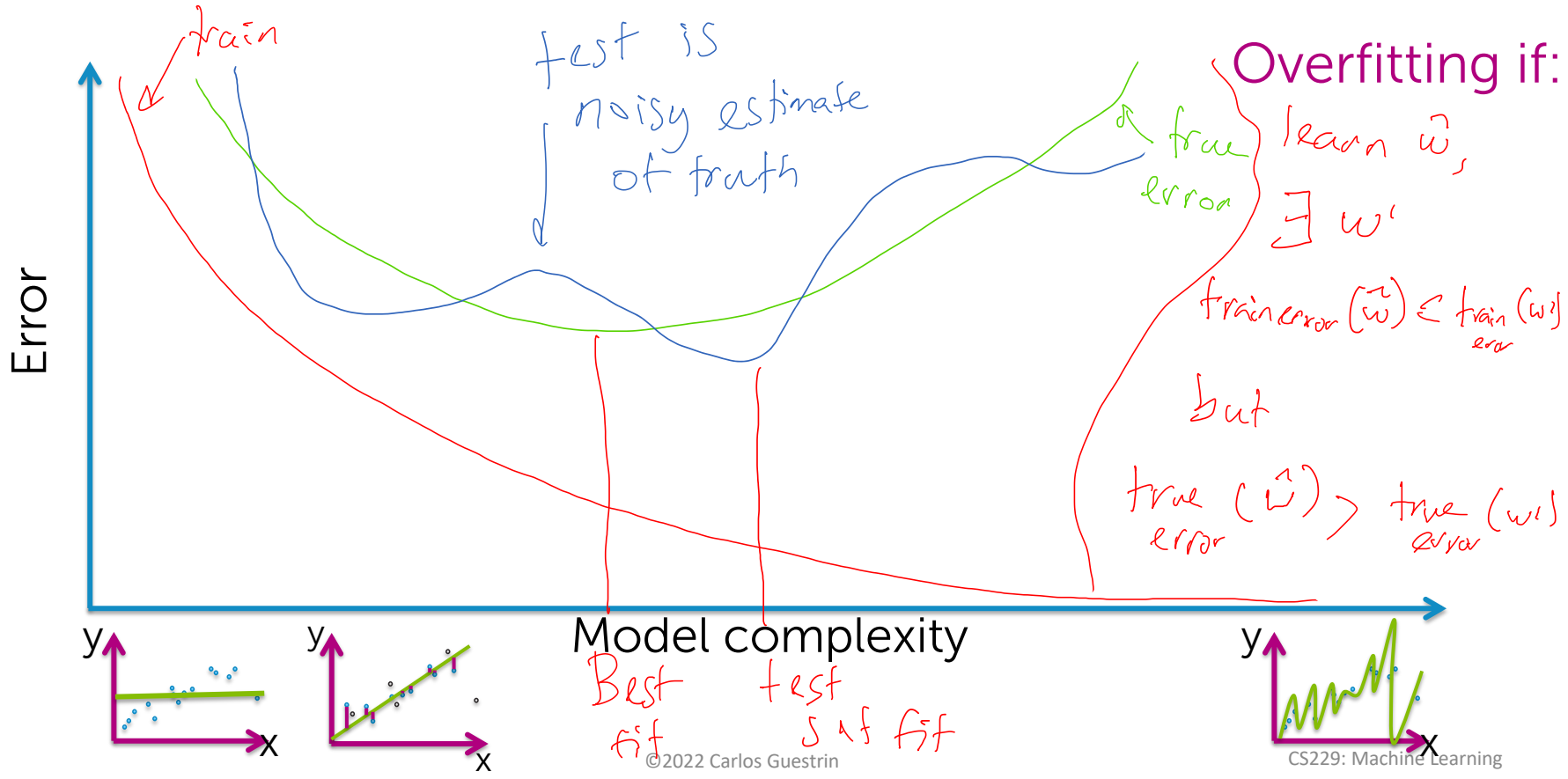


True error vs. model complexity



Assessing the loss
Part 3: Test error

Training, true, test error vs. model complexity



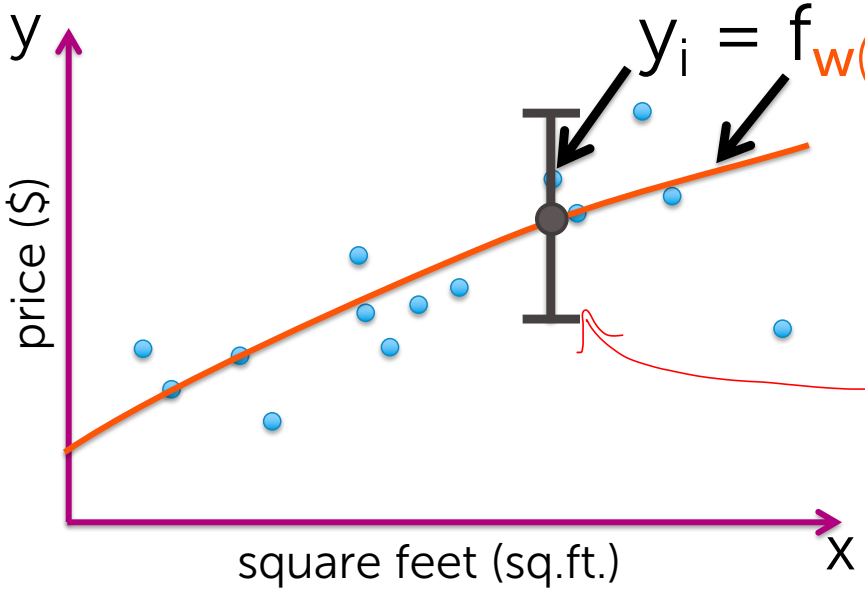
3 sources of error + the bias-variance tradeoff

3 sources of error

In forming predictions, there are 3 sources of error:

1. Noise
2. Bias ← how well can model fit data on avg.
3. Variance ← how much model would change if I change dataset samples

Data inherently noisy



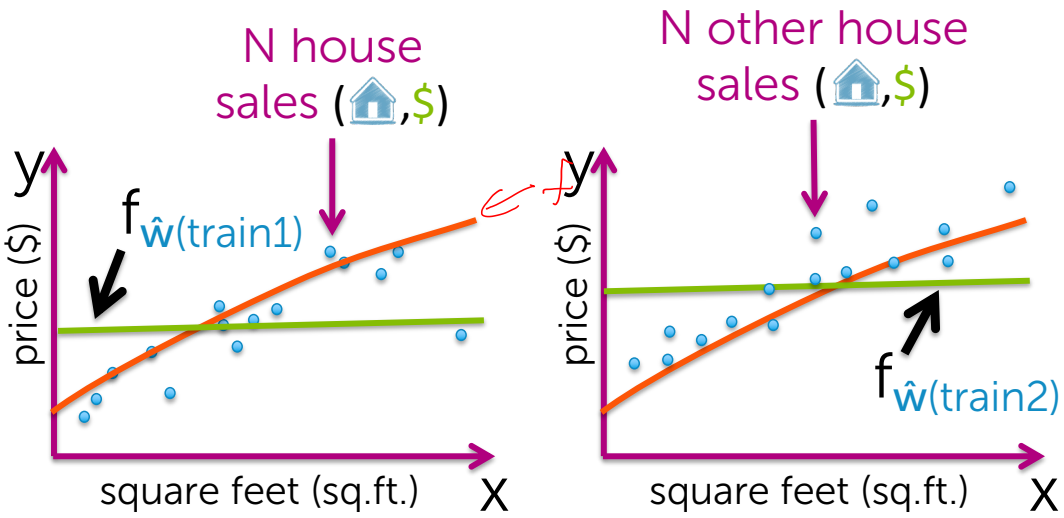
$$y_i = f_{w(true)}(x_i) + \varepsilon_i$$

independent
zero mean noise

unavoidable loss

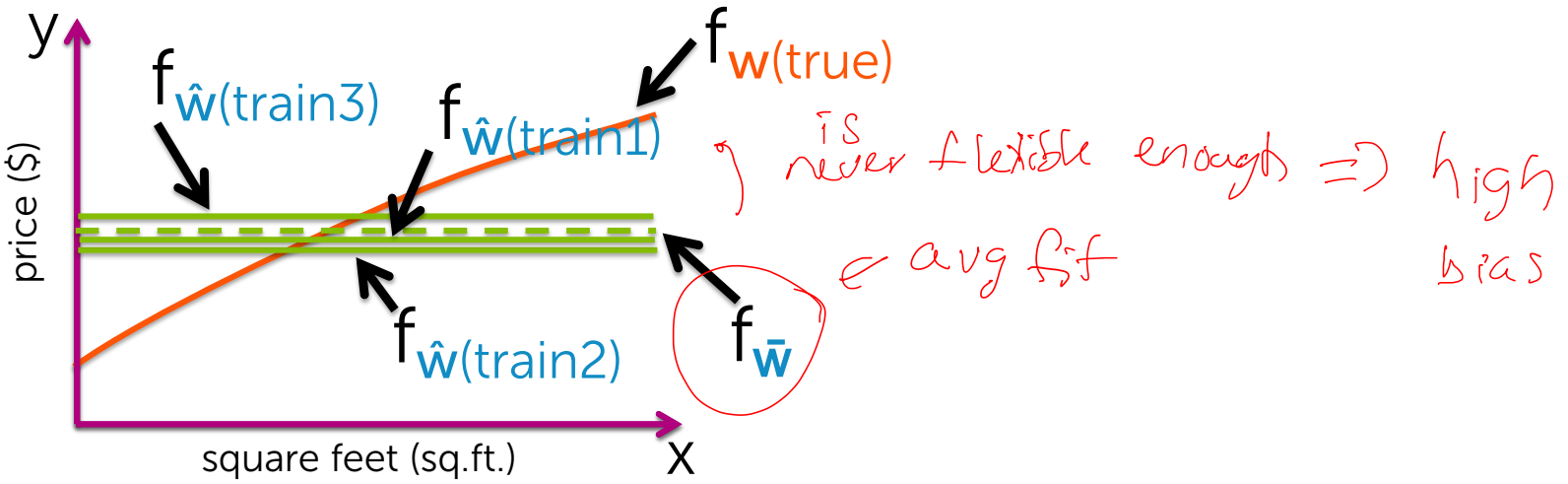
Bias contribution

Suppose we fit a constant function



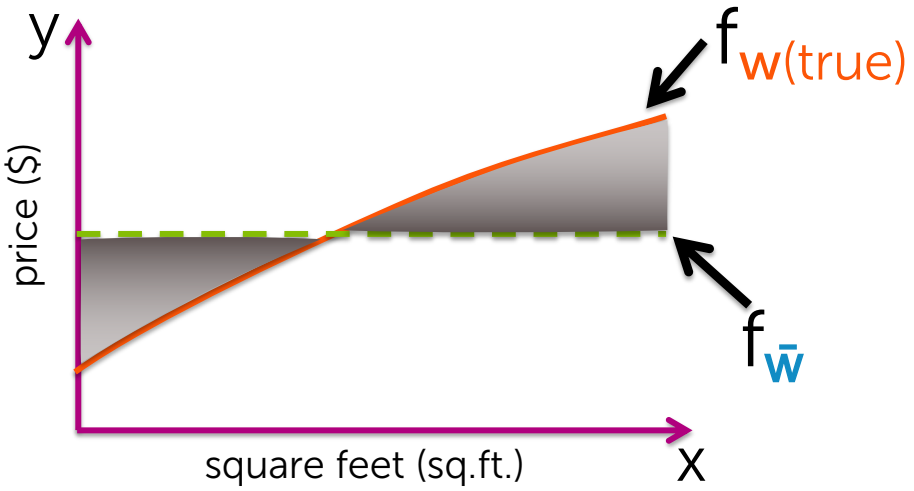
Bias contribution

Over all possible size N training sets,
what do I expect my fit to be?



Bias contribution

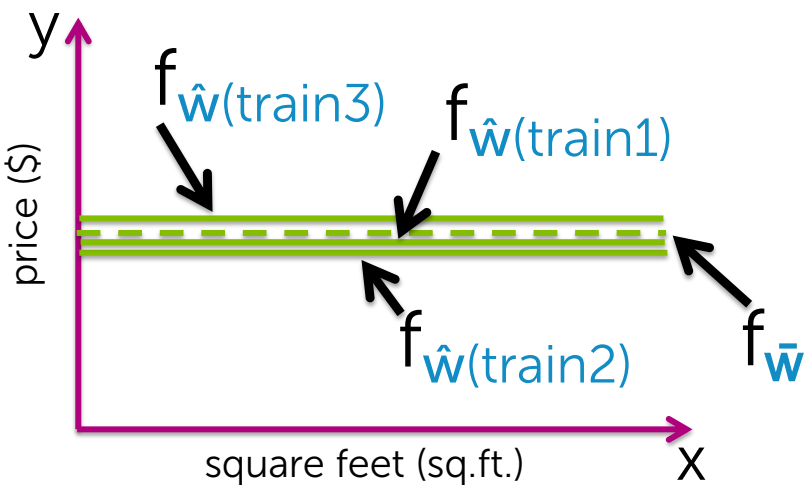
$\text{Bias}(\mathbf{x}) = f_{\mathbf{w}(\text{true})}(\mathbf{x}) - f_{\bar{\mathbf{w}}}(\mathbf{x})$ ← Is our approach flexible enough to capture $f_{\mathbf{w}(\text{true})}$? **If not, error in predictions.**



low complexity → high bias

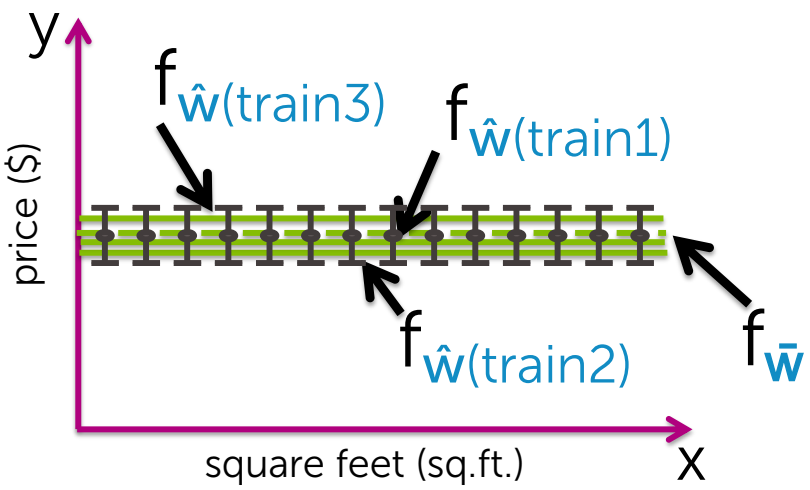
Variance contribution

How much do specific fits vary from the expected fit?



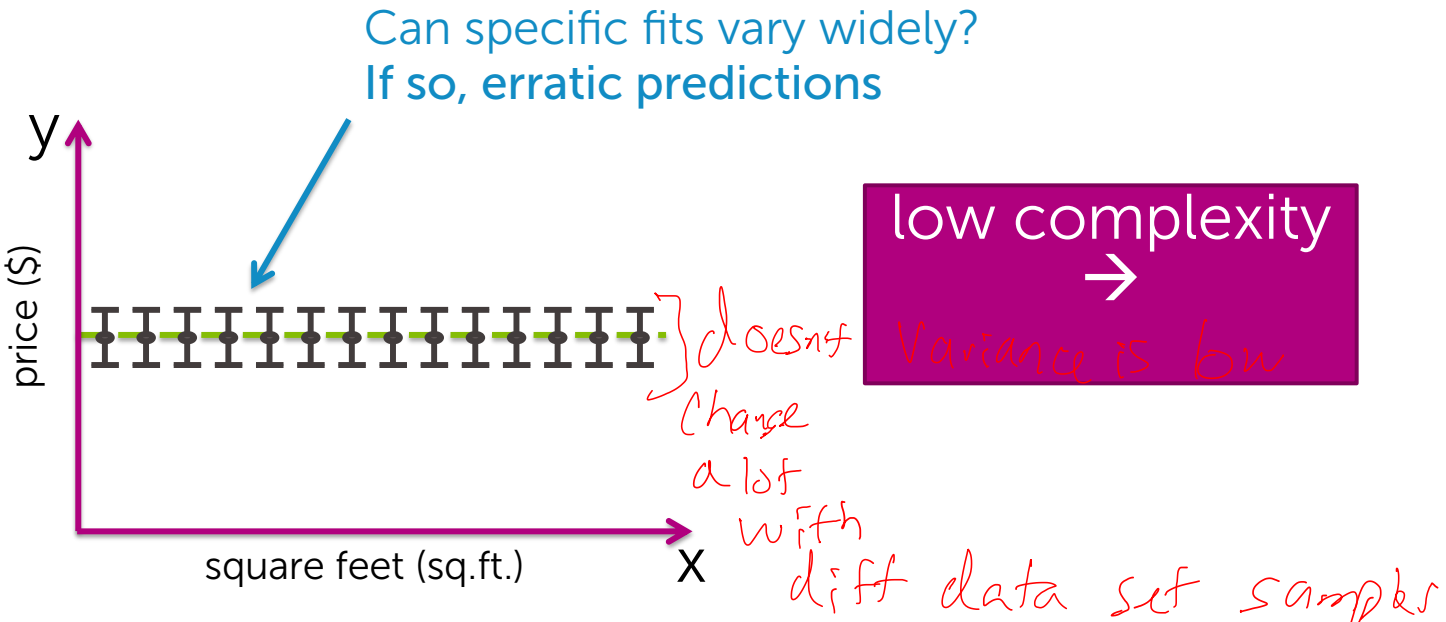
Variance contribution

How much do specific fits vary from the expected fit?



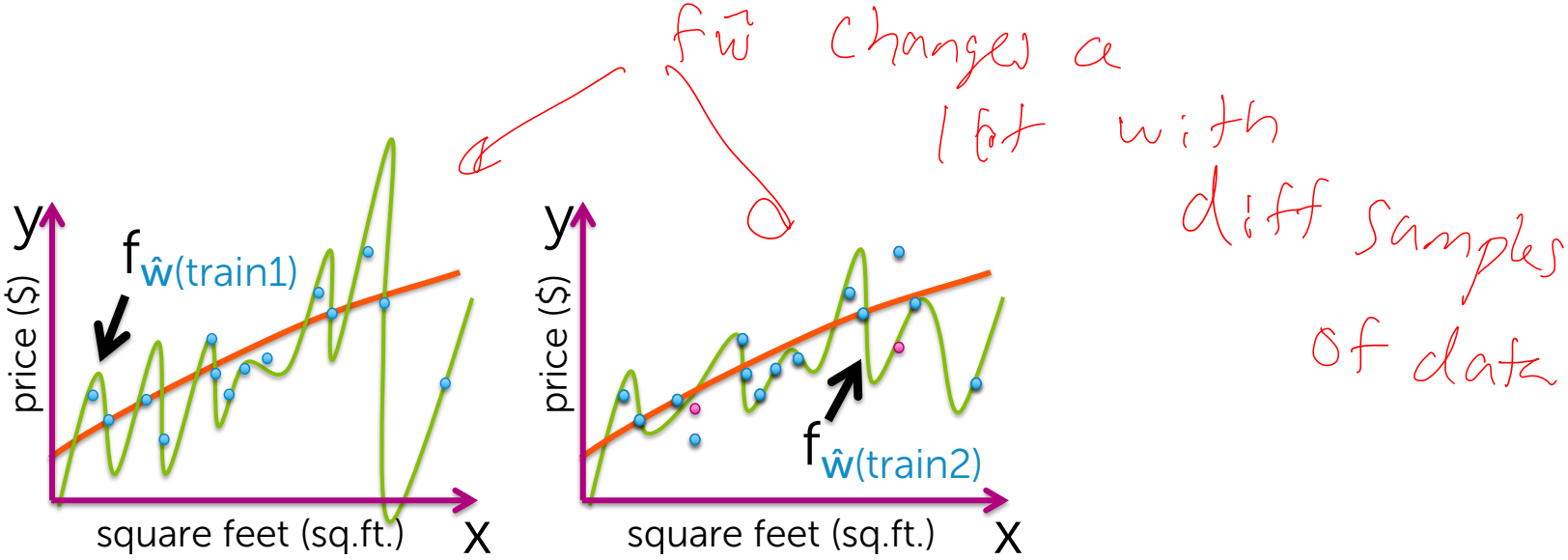
Variance contribution

How much do specific fits vary from the expected fit?



Variance of high-complexity models

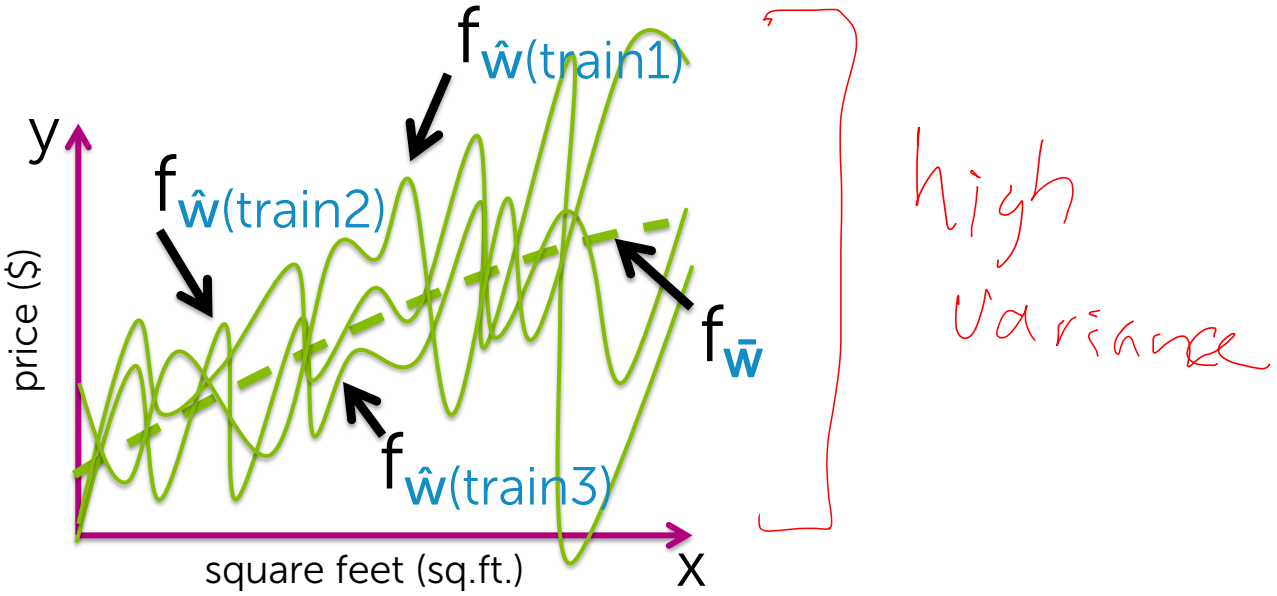
Assume we fit a high-order polynomial



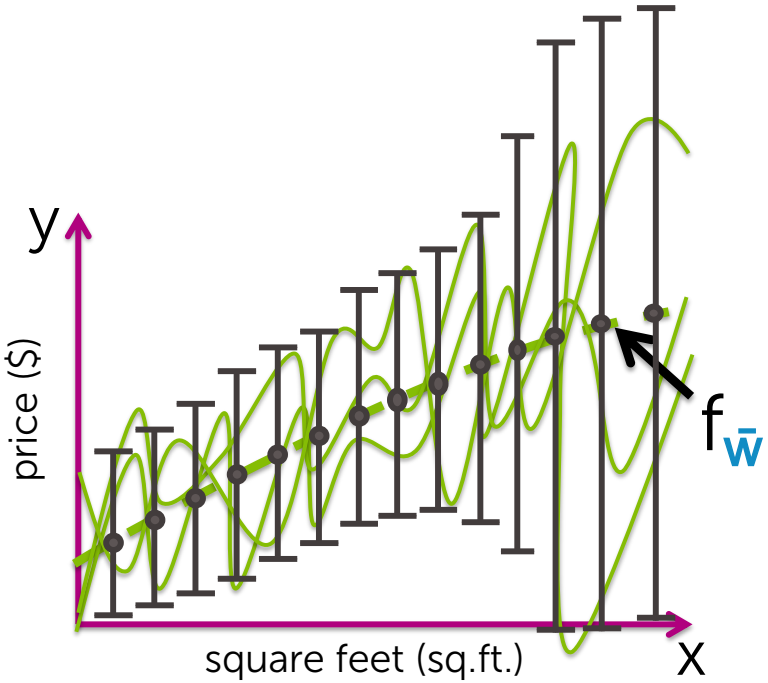
$f_{\hat{w}}$ changes a lot with diff samples of data

Variance of high-complexity models

Suppose we fit a high-order polynomial

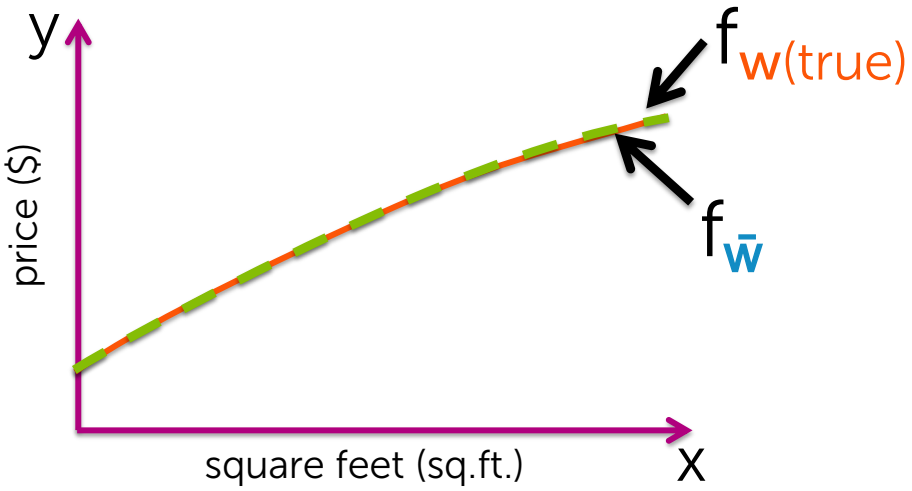


Variance of high-complexity models



high complexity
→
high variance

Bias of high-complexity models

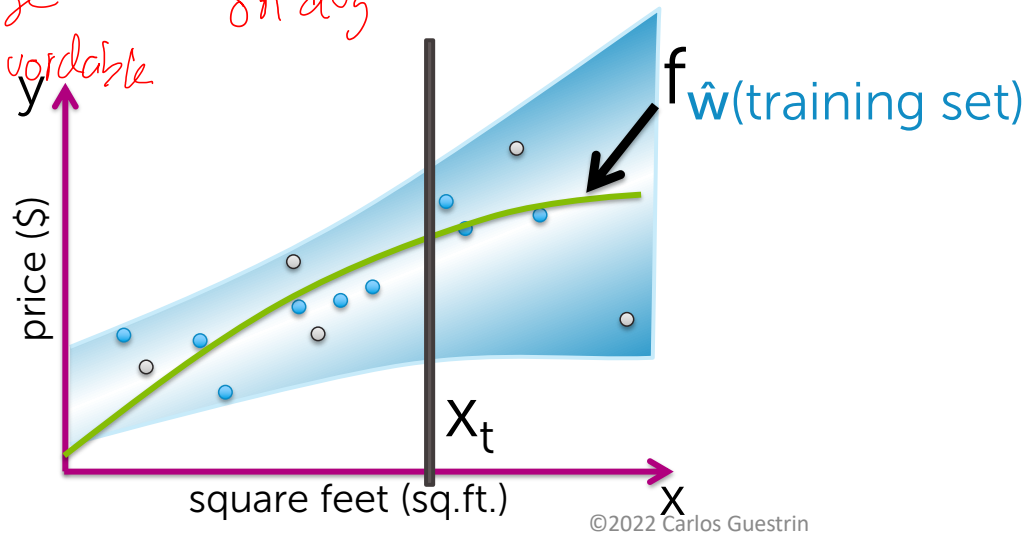


high complexity
→
low bias

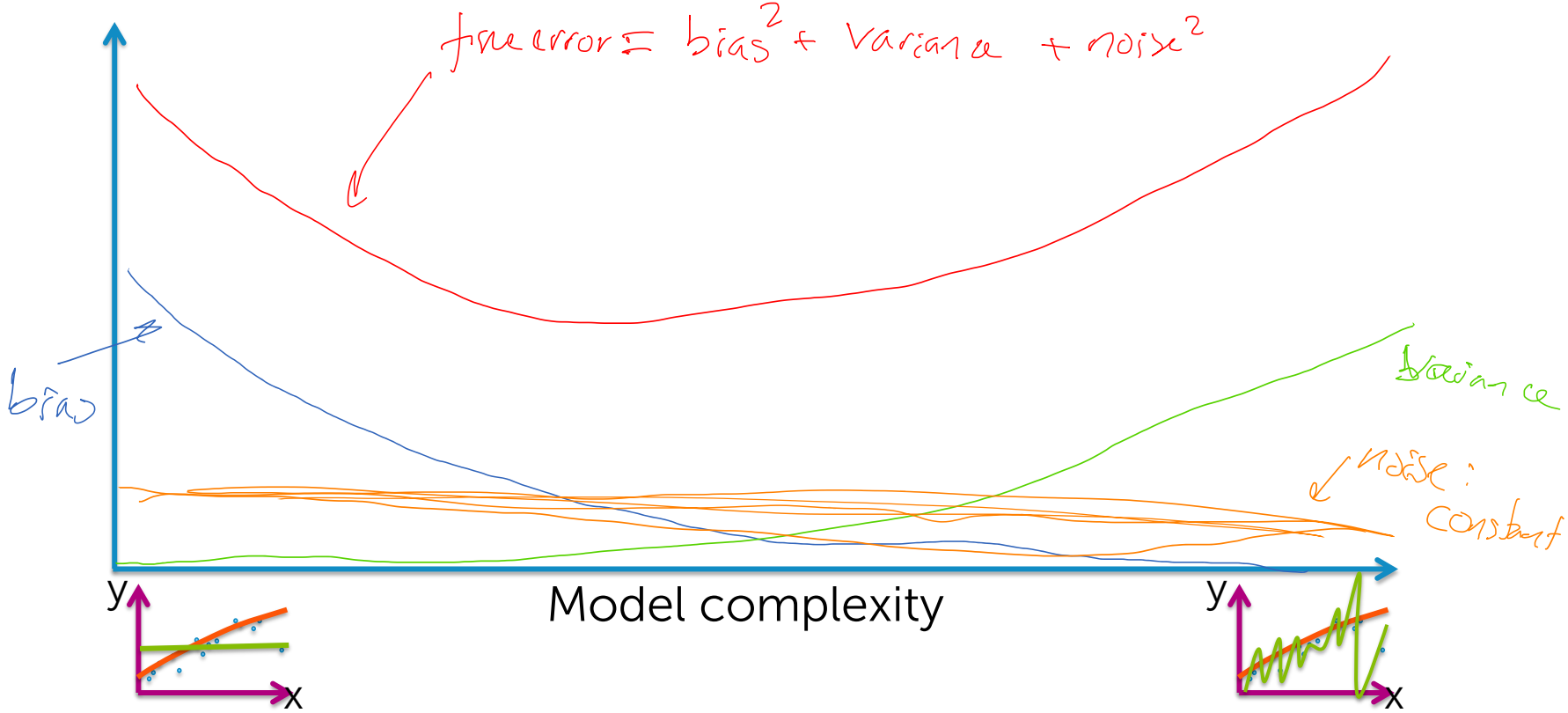
Sum of 3 sources of error

Average squared error at x_t

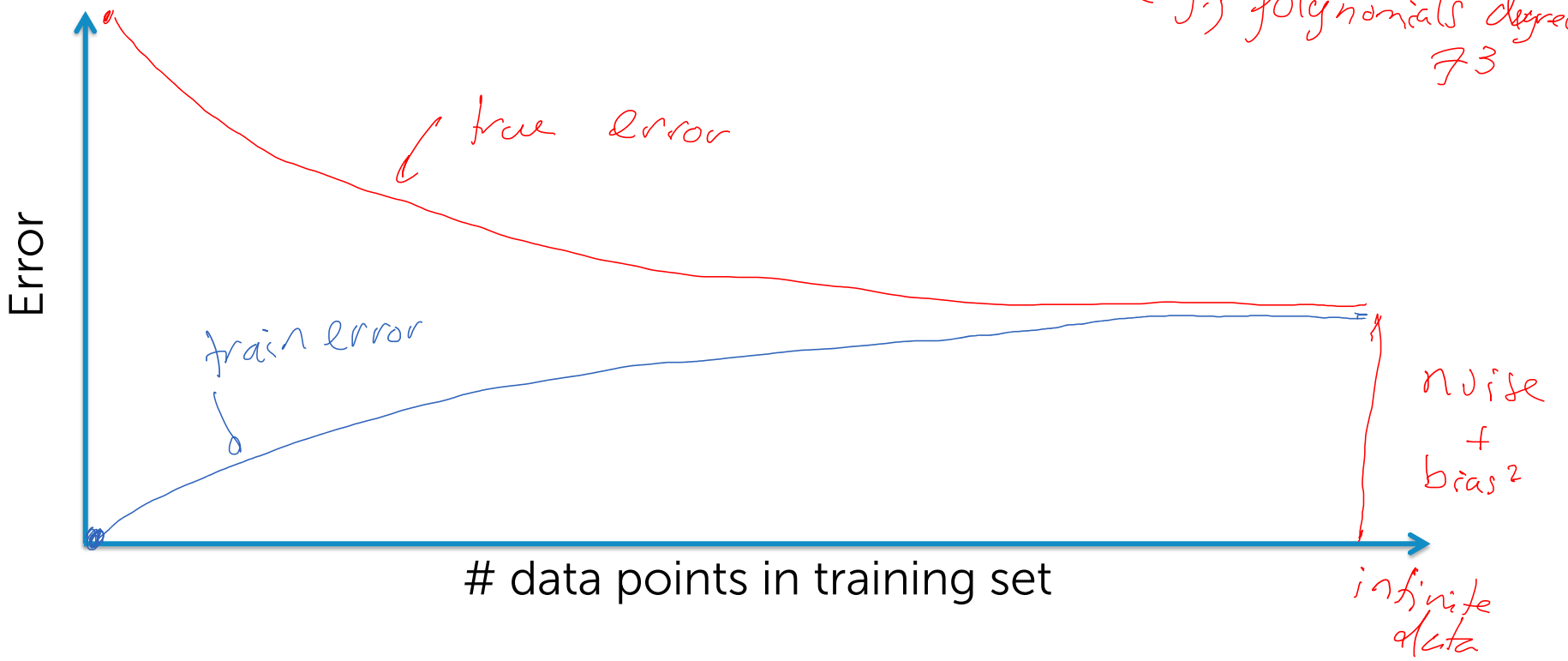
$$= \sigma^2 + [\text{bias}(f_{\hat{w}}(x_t))]^2 + \text{var}(f_{\hat{w}}(x_t))$$



Bias-variance tradeoff



Error vs. amount of data



Why 3 sources of error?
A formal derivation

Deriving expected prediction error

Expected prediction error

$= E_{train}$ [generalization error of $\hat{\mathbf{w}}(train)$]

$= E_{train}\left[E_{\mathbf{x},y}[L(y, f_{\hat{\mathbf{w}}(train)}(\mathbf{x}))]\right]$

1. Look at specific $\mathbf{x}_t$
2. Consider $L(y, f_{\hat{\mathbf{w}}}(\mathbf{x})) = (y - f_{\hat{\mathbf{w}}}(\mathbf{x}))^2$

Expected prediction error at $\mathbf{x}_t$

$= E_{train, y_t}[(y_t - f_{\hat{\mathbf{w}}(train)}(\mathbf{x}_t))^2]$

Simplifying Notation

- Expected prediction error at $\mathbf{x}_t$

  $= E_{\text{train},y_t}\left[(y_t - f_{\hat{\mathbf{w}}(\text{train})}(\mathbf{x}_t))^2\right]$

- Simple (and abusive ☺) notation:
  - $y_t \rightarrow y$
  - $f_{\mathbf{w}(\text{true})}(\mathbf{x}_t) \rightarrow f$ ← true
  - $f_{\hat{\mathbf{w}}(\text{train})}(\mathbf{x}_t) \rightarrow \hat{f}$ ← learned
  - $E_{\text{train}}\left[f_{\hat{\mathbf{w}}(\text{train})}(\mathbf{x}_t)\right] = f_{\bar{\mathbf{w}}}(\mathbf{x}_t) \rightarrow \bar{f}$ learned on avg.

Deriving expected prediction error

$E[ab] = E[a]\,E[b]$ (a, b independent)

Expected prediction error at x_t

$$= E_{train, y_t}[(y_t - f_{\hat{w}(train)}(x_t))^2] = E_{train}[(y - \hat{f})^2] =$$

$$= E_{train}[((y - f) + (f - \hat{f}))^2]$$

$$= E[(y-f)^2] + 2\,E_{train}[(y-f)(f-\hat{f})] + E_{train}[(f-\hat{f})^2]$$

$E[(y-f)^2]$: by definition: noise σ^2

$E_{train}[(y-f)(f-\hat{f})] = E_{train}[(y-f)]\,E_{train}[(f-\hat{f})]$; $(y-f)$: zero mean noise

$E_{train}[(f-\hat{f})^2] \triangleq MSE(\hat{f})$ mean squared error

$$= \sigma^2 + MSE(\hat{f})$$

Equating MSE with bias and variance

$$\text{MSE}[f_{\hat{w}(\text{train})}(x_t)]$$

$$= E_{\text{train}}[(f - \hat{f})^2]$$

$$= E_{\text{train}}[((f - \bar{f}) + (\bar{f} - \hat{f}))^2]$$

$$= E_{\text{train}}[(f-\bar{f})^2] + 2E_{\text{train}}[(f-\bar{f})(\bar{f}-\hat{f})] + E_{\text{train}}[(\bar{f}-\hat{f})^2]$$

$= 0$

mean, random var.

by defn. bias^2

$2E_{\text{train}}[(f-\bar{f})]\,E_{\text{train}}[\bar{f}-\hat{f}]$ (if)

$E[\bar{f}] - E[\bar{f}]$

$= \text{Var}(\hat{f})$

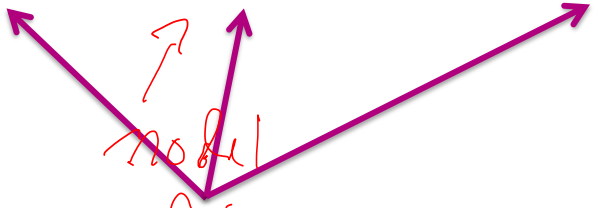
$$= \text{bias}^2 + \text{Var}$$

Putting it all together

Expected prediction error at $\mathbf{x}_t$

$$= \sigma^2 + \text{MSE}\left[f_{\hat{\mathbf{w}}}(\mathbf{x}_t)\right]$$

$$= \sigma^2 + \left[\text{bias}(f_{\hat{\mathbf{w}}}(\mathbf{x}_t))\right]^2 + \text{var}(f_{\hat{\mathbf{w}}}(\mathbf{x}_t))$$



3 sources of error

flexibility of the model

Summary of bias-variance tradeoff

What you can do now…

- Contrast relationship between model complexity and train, true and test loss
- Compute training and test error given a loss function for different model complexities
- List and interpret the 3 sources of avg. prediction error
  - Irreducible error, bias, and variance